Appendix I-2 Chemical Risk Assessment Tables

Register of Assessed Chemicals

Santos

Chemical Name	CAS No.	Document Control					Overall PBT Assessment [2]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Tier [4]	Risk Level
		Chemical Assessment Date	Independent Peer Reviewer [1]	Department Notification Date	Department Approval Date	Chemical Re-evaluation Date		Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [3]	Chronic Toxicity [3]		
1,3-Dichloropropene	542-75-6	12/21/2022	NA	NA	-	-	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA [5]	Low
2,2-Dibromo-3-Nitrilopropionamide (DBNPA)	10222-01-2	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	3	3	3	High
2-Mercaptoethanol	60-24-2	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	1 (fish and algae), 3 (invert)	2	2	Low
2-Propenoic acid, potassium salt, polymer with 2-propenamide	31212-13-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1 [4]	Low
2-Propenoic acid, sodium salt, polymer with 2-propenamide	25085-02-3	12/9/2020	NA	NA	-	-	Not a PBT	No	Yes	Yes	No	No	No	1	1	1	Low
3,5,7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane,1-(3-chloro-2-propenyl)- , chloride (CTAC)	4080-31-3	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	No data	2	Low
5-chloro-2-methyl-4-isothiazolin-3-one and 2-methyl-4-isothiazolin-3-one (CMIT/MIT)	55965-84-9	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	3	3	3	High
Acetic Acid	64-19-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Acetylene	74-86-2	10/28/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	No data	1	Low
Acrylamide, sodium acrylate polymer	25987-30-8	12/9/2020	NA	NA	-	-	Not a PBT	No	Yes	Yes	No	No	No	1	1	1 [4]	Low
Acrylate Terpolymer	903573-39-7	12/21/2022	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Alcohols, C12-15, ethoxylated	68131-39-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Alcohols, C12-16, ethoxylated	68551-12-2	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2 (fish), 3 (inv and algae)	2	2	Low
Aliphatic alcohol ethoxylate	9004-77-7	4/16/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Alkanes, C11-15-iso-	90622-58-5	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	2	2	Low
Aluminum Hydroxychloride	1327-41-9	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	Yes	3	3	3	High
Aluminum oxide	1344-28-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Amides, coco, N,N-bis (hydroxyethyl)	68603-42-9	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	No data	2	Low
Amides, tall-oil fatty, N,N-bis(hydroxyethyl)	68155-20-4	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	2	2	2	Low
Amine Oxides, cocoalkyldimethyl	61788-90-7	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	2 (Fish & Inv), 3 (Algae)	2 (Fish & Inv), 3 (Algae)	2	Low
Ammonium hydroxide	1336-21-6	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	2	2	2	Low
Amylodextrin	9005-84-9	10/28/2021	NA	NA	-	-	Not a PBT	No	Yes	No	No	No	No	1	No data	1	Low
Barium Sulfate	7727-43-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Bentonite	1302-78-9	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Benzaldehyde	100-52-7	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2 (Fish & Algae), 1 (Inv)	2 (Fish), 1 (Algae)	2	Low
Benzenesulfonic acid, dimethyl-, sodium salt	1300-72-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Benzyl-C1-2-alkylpyridinium chloride	68909-18-2	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	2	No Data	2	Low
Boric acid	10043-35-3	12/21/2022	NA	NA	-	-	Not a PBT	Yes	No	NA	No	No	No	1	1	2	Low
but-2-enedioic acid	110-17-8	9/1/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Butyl alcohol	71-36-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
C10-C16 Alkylbenzenesulfonic acid	68584-22-5	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	Insufficient data quality for categorisation	2	Low
Calcined petroleum coke	64743-05-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	Will either incorporate into sediment or float to the surface.	No	No	1	1	1	Low
Calcium carbide	75-20-7	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	2	No data	2	Low
Calcium Carbonate	471-34-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Calcium Chloride	10043-52-4	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Calcium Hydroxide	1305-62-0	4/16/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Calcium lignosulfonate	8061-52-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Calcium Oxide	1305-78-8	4/16/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Castor Oil	8001-79-4	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Cellophane	9005-81-6	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Cellulase enzyme	9012-54-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Chlorous acid, sodium salt (or sodium chlorite)	7758-19-2	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1 (Fish), 3 (Algae)	No data	2	Low
Choline Chloride	67-48-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Cinnamaldehyde	104-55-2	7/26/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2 (Fish & Inv), 1 (Algae)	1 (Fish), 2 (Inv)	1	Low
Citric Acid	77-92-9	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Cocamidopropyl betaine	61789-40-0	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	2	2	Low
Cocoalkyl dimethylbenzyl ammonium chloride (ADBAC)	61789-71-7	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	3	3	3	High
Coffee Extract	68916-18-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Cupric Nitrate	3251-23-8	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	Yes	3	3	3	High
Dialuminium Chloride Pentahydroxide	12042-91-0	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	Yes	3	1	3	High
Diammonium peroxidisulphate	7727-54-0	12/2/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Dichloromethane (methylene chloride)	75-09-2	12/21/2022	NA	NA	-	-	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA [5]	Low
Diethanolamine	111-42-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Diethylene Glycol	111-46-6	7/26/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Diethylene glycol monobutyl ether	112-34-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane)	27306-78-1	7/26/2021	NA	NA	-	-	Not a PBT	No	Yes	No	No	No	No	1	1	1	Low
Disodium disulphite	7681-57-4	12/2/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Disodium metasilicate	6834-92-0	4/13/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Disodium octaborate tetrahydrate	12008-41-2	7/26/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Diutan	595585-15-2	12/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1 [4]	Low
Diutan Gum	125005-87-0	12/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1 [4]	Low
Ethanol	64-17-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Ethanol, 2,2'-oxybis-, reaction products with ammonia,morpholine derivatives residues	68909-77-3	4/16/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Ethoxylated alcohol	78330-21-9	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2 (fish) and 3 (inverts and algae)	2	2	Low
Ethyl hexanol	104-76-7	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	2	2	Low
Ethylene glycol	107-21-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Ethylene glycol monobutyl ether	111-76-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Ethylene oxide / propylene oxide copolymer	9082-00-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1 [4]	Low
Ethylene oxide / propylene oxide copolymer	9003-11-6	12/9/2020	NA	NA	-	-	Not a PBT	No	Yes	No	No	No	No	1	1	1	Low
Fatty Acid Ester	10024-47-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Fatty Acids Ester	135800-37-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Fatty acids, tall-oil, ethoxylated	61791-00-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Food red 10	3734-67-6	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Formic Acid	64-18-6	6/20/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Gelatins	9000-70-8	12/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	No data	No data	1	Low
Glass, oxide	65997-17-3	7/26/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Glutaraldehyde	111-30-8	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	2 (fish & inverts), 3 (algae)	2	3	High
Glycerine	56-81-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Glyoxal	107-22-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Graphite	7782-42-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Guar gum	9000-30-0	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	Potentially Yes	1	1	1	Low
Hemicellulase enzyme	9025-56-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Heterocyclic polymer containing nitrogen compounds	9003-39-8	4/16/2021	NA	NA	-	-	Not a PBT	No	Yes	No	No	No	No	1	1	1	Low
Hexamethylenediamine	124-09-4	7/26/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Hexamethylenetetramine	100-97-0	12/21/2022	NA	NA	-	-	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA [5]	Low
Hexanedinitrile	111-69-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	64742-47-8	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	2	2	Low
Hydrochloric Acid	7647-01-0	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1 (fish), 3 (algae & inverts) (ECHA)	No Data	3	High
Hydrogen Peroxide	7722-84-1	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	3	2d	Low
Hydroxylpropyl guar	39421-75-5	6/20/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	Potentially Yes	1	No data	1	Low

Santos

Chemical Name	CAS No.	Document Control					Overall PBT Assessment [2]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Tier [4]	Risk Level
		Chemical Assessment Date	Independent Peer Reviewer [1]	Department Notification Date	Department Approval Date	Chemical Re-evaluation Date		Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [3]	Chronic Toxicity [3]		
Iron oxide	1309-37-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Isopropanol	67-63-0	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Isotridecanol, ethoxylated	69011-36-5	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	2	2	2	Low
Lactose	63-42-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Lecithins	8002-43-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Magnesium chloride	7786-30-3	9/1/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Magnesium nitrate	10377-60-3	9/1/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Magnesium oxide	1309-48-4	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Magnesium silicate hydrate (talc)	14807-96-6	12/2/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	No data	1	Low
Melamine, formaldehyde, sodium bisulfite polymer	64787-97-9	12/9/2020	NA	NA	-	-	Not a PBT	No	Yes	No	No	No	No	1	1	1	Low
Methanol	67-56-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Methyl Acetate	79-20-9	6/20/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Mixture of dimer and trimer fatty acids of indefinite composition derived from tall oil	61790-12-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Modified bentonite	71011-24-0	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Monoethanolamine	141-43-5	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1 (fish, inv) 2 (algae)	1 (fish), 2 (inv, algae)	2	Low
Monoethanolamine borate	26038-87-9	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
N,N-Dimethylmethanamine	75-50-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Nitrilotriacetic acid, trisodium salt monohydrate	5064-31-3	4/16/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Nitrogen	7727-37-9	7/27/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Organic Derivative of Phosphonic Acid, K Salt	38820-59-6	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Oxazolidine	66204-44-2	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1 (fish, inv) 2 (algae)	1	2	Low
Peroxyacetic Acid	79-21-0	12/21/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	3	3	3	High
Poly(vinyl acetate)-poly(vinyl alcohol) polymer	25213-24-5	6/20/2021	NA	NA	-	-	Not a PBT	No	Yes	Yes	No	No	No	1	1	1	Low
Polyalkylene Glycol Monobutyl Ether	9038-95-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
PolyDADMAC	26062-79-3	12/21/2022	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	2	2	2	Low
Polyethylene glycol	25322-68-3	12/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Polypropylene	9003-07-0	12/9/2020	NA	NA	-	-	Not a PBT	No	Yes	Yes	No	No	No	1	1	1[f]	Low
Polypropylene Glycol	25322-69-4	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Polyquaternium-33	69418-26-4	12/21/2022	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	2	2	2	Low
Polyurethane foam	9009-54-5	8/29/2022	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	No Data	1	Low
Portland Cement	65997-15-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Potassium borate	1332-77-0	12/2/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Potassium Carbonate	584-08-7	12/2/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	No Data	1	Low
Potassium Chloride	7447-40-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Potassium Hydroxide	1310-58-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Potassium pyrophosphate	7320-34-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Potassium Sulphate	7778-80-5	6/20/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	No data	1	Low
Silicic Acid, Potassium Salt	1312-76-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Silicon dioxide	112926-00-8	6/20/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Silicon dioxide	7631-86-9	6/20/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Silicon dioxide	112945-52-5	6/20/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Silicone based emulsion neutralised polyacrylic based stabiliser	NS	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1[a]	Low
Sodium Acetate	127-09-3	6/20/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Sodium Acid Pyrophosphate	7758-16-9	4/16/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Bicarbonate	144-55-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Bromide	7647-15-6	12/2/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Carbonate	497-19-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Sodium Carboxymethylcellulose	9004-32-4	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Sodium Chloride	7647-14-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Dodecyl Sulfate	151-21-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Sodium Erythorbate	6381-77-7	4/16/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Sodium gluconate	527-07-1	12/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Sodium Hydroxide	1310-73-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Hypochlorite	7681-52-9	12/21/2022	NA	NA	-	-	Not a PBT	No	No	NA	No	No	Yes	3	3	3	High
Sodium Iodide	7681-82-5	6/20/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium lauryl polyoxyethylene ether sulfate	9004-82-4	7/26/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Sodium lignosulfonate	8061-51-6	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Sodium nitrite	7632-00-0	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	2	1	1[g]	Low
Sodium persulfate	7775-27-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Polyacrylate	9003-04-7	12/9/2020	NA	NA	-	-	Not a PBT	No	Yes	Yes	No	No	No	1	1	1	Low
Sodium polynaphthalene sulfonate	9008-63-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Sodium silicate	1344-09-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Sulfate	7757-82-6	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium sulphite	7757-83-7	6/20/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sodium Tetraborate Decahydrate (Borax)	1303-96-4	12/21/2022	NA	NA	-	-	Not a PBT	Yes	No	NA	No	No	No	1	1	2	Low
Sodium thiosulphate	7772-98-7	9/3/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Sorbitan monolaurate, ethoxylated	9005-64-5	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Sorbitan, mono-9-octadecenoate, (Z)	1338-43-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Sorbitan, mono-9-octadecenoate, ploy(oxy-1,2-ethanediyl) derivatives, (Z)	9005-65-6	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Soybean oil	8001-22-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Soybean oil, methyl ester, sulfated, sodium salt	68918-47-8	8/29/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Starch	9005-25-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Starch, carboxymethyl ether	9057-06-01	10/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Starch, polymer with (chloromethyl)oxirane	58944-89-1	6/20/2021	NA	NA	-	-	Not a PBT	No	Yes	No	No	No	No	1	1	1	Low
Sulfated oleic acid, potassium salt	68473-93-8	8/29/2022	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No Data	1	Low
Tetramethyl ammonium chloride	75-57-0	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	Yes	1	3	1[g]	Low
Tributyl tetradecyl phosphonium chloride	81741-28-8	12/21/2022	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	Yes	3	3	3	High
Triethanolamine	102-71-6	7/26/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Trimethylamine hydrochloride	593-81-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No data	1	Low
Trisodium Citrate	68-04-2	12/2/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	No Data	1	Low
Ulexite	1319-33-1	7/26/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1	Low
Vinylamide/vinyl sulfonated polymer	110897-64-8	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Vinylidene chloride/methylacrylate copolymer	25038-72-6	9/1/2021	NA	NA	-	-	Not a PBT	No	Yes	Yes	No	No	No	1	1	1	Low
Water (in Products)	7732-18-5	6/20/2021	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1	Low
Xanthan Gum	11138-66-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	Yes	No	No	No	1	1	1	Low
Silica																	
Crystalline silica, cristobalite	14464-46-1	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1[h]	Low
Crystalline silica, quartz	14808-60-7	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1[h]	Low
Crystalline silica, tridymite	15468-32-3	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1[h]	Low
Diatomaceous earth	61790-53-2	12/9/2020	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1[h]	Low
Non-crystalline silica (impurity)	7631-86-9	11/3/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1[h]	Low
Diatomaceous earth, calcined	91053-39-3	11/3/2021	NA	NA	-	-	Not a PBT	No	No	NA	No	No	No	1	1	1[h]	Low

Register of Assessed Chemicals

Chemical Name	CAS No.	Document Control					Overall PBT Assessment [2]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Tier [4]	Risk Level
		Chemical Assessment Date	Independent Peer Reviewer [1]	Department Notification Date	Department Approval Date	Chemical Re-evaluation Date		Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [3]	Chronic Toxicity [3]		
Wood Products																	
Almond Hulls	NS	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1[i]	Low
Nut Hulls	Mixture	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1[i]	Low
Vegetable Fibre	NS	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1[i]	Low
Walnut hulls	Mixture (1756)	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1[i]	Low
Wood fiber	Mixture (1757)	12/9/2020	NA	NA	-	-	Not a PBT	No	No	No	No	No	No	1	1	1[i]	Low

Footnotes:

1 - Only required for new Tier 1 and Tier 2 chemicals

2 = PBT Assessment based on PBT Framework.

3 = Acute and chronic aquatic toxicity evaluated consistent with assessment criteria and framework.

4 = Categorisation as defined in assessment framework.

a - Similar polymers grouped together. See assessment for CAS NO.25085-02-3

b - Impurities present at de minimus levels. See assessment for CAS NO. 4080-31-3

c - Similar polymers grouped together. See assessment for CAS NO. 9003-11-6

d - Preponderance of data indicates appropriateness of Tier 2. See dossier for more information.

f - Similar polymers grouped together. See assessment for CAS NO. 25322-69-4

g - Preponderance of data indicates appropriateness of Tier 1. See dossier for more information.

h - Similar chemicals grouped together. See assessment for 14464-46-1/14808-60-7/15468-32-3/61790-53-2/7631-86-9/91053-39-3

i - Similar chemicals grouped together. Assessment for wood products includes almond hulls, nut hulls, walnut hulls, vegetable fibre and wood fibre

k - Similar chemicals grouped together. See assessment for 595585-15-2/125005-87-0

Notes:

NA = not applicable

NR = not required

NS = not supplied

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

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Chemical Name	CAS No.	Assessed Activity(ies)			Assessed Use(s)					
		Drilling and Completions	Hydraulic Fracturing	Water Treatment	Residual Drilling Material	Irrigation	Stockwatering	Surface Water	Dust Supression/ Construction	TBA
1,3-Dichloropropene	542-75-6	X			X	X	X	X	X	
2,2-Dibromo-3-Nitrilopropionamide (DBNPA)	10222-01-2			X				X		
2-Mercaptoethanol	60-24-2			X				X		
2-Propenoic acid, potassium salt, polymer with 2-propenamide	31212-13-2	X			X	X	X	X	X	
2-Propenoic acid, sodium salt, polymer with 2-propenamide	25085-02-3	X			X	X	X	X	X	
3,5,7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane,1-(3-chloro-2-propenyl)- , chloride (CTAC)	4080-31-3	X						X		
5-chloro-2-methyl-4-isothiazolin-3-one and 2-methyl-4-isothiazolin-3-one (CMIT/MIT)	55965-84-9		X	X				X		
Acetic Acid	64-19-7		X	X		X	X	X	X	
Acetylene	74-86-2	X			X	X	X	X	X	
Acrylamide, sodium acrylate polymer	25987-30-8	X			X	X	X	X	X	
Acrylate Terpolymer	903573-39-7			X		X	X	X	X	
Alcohols, C12-15, ethoxylated	68131-39-5		X			X	X	X	X	
Alcohols, C12-16, ethoxylated	68551-12-2		X					X		
Aliphatic alcohol ethoxylate	9004-77-7	X			X	X	X	X	X	
Alkanes, C11-15-iso-	90622-58-5	X						X		
Aluminum Hydroxychloride	1327-41-9			X				X		
Aluminum oxide	1344-28-1	X			X	X	X	X	X	
Amides, coco, N,N-bis (hydroxyethyl)	68603-42-9	X						X		
Amides, tall-oil fatty, N,N-bis(hydroxyethyl)	68155-20-4		X					X		
Amine Oxides, cocoalkyldimethyl	61788-90-7		X					X		
Ammonium hydroxide	1336-21-6			X				X		
Amylodextrin	9005-84-9	X			X	X	X	X	X	
Barium Sulfate	7727-43-7	X			X	X	X	X	X	
Bentonite	1302-78-9	X			X	X	X	X	X	
Benzaldehyde	100-52-7		X					X		
Benzenesulfonic acid, dimethyl-, sodium salt	1300-72-7	X			X	X	X	X	X	
Benzyl-C1-2-alkylpyridinium chloride	68909-18-2			X				X		
Boric acid	10043-35-3		X					X		
but-2-enedioic acid	110-17-8		X			X	X	X	X	
Butyl alcohol	71-36-3		X			X	X	X	X	
C10-C16 Alkylbenzenesulfonic acid	68584-22-5	X						X		
Calcined petroleum coke	64743-05-1	X			X	X	X	X	X	
Calcium carbide	75-20-7	X						X		
Calcium Carbonate	471-34-1	X			X	X	X	X	X	
Calcium Chloride	10043-52-4	X			X	X	X	X	X	
Calcium Hydroxide	1305-62-0	X			X	X	X	X	X	
Calcium lignosulfonate	8061-52-7	X			X	X	X	X	X	
Calcium Oxide	1305-78-8	X			X	X	X	X	X	
Castor Oil	8001-79-4	X			X	X	X	X	X	
Cellophane	9005-81-6	X			X	X	X	X	X	
Cellulase enzyme	9012-54-8		X			X	X	X	X	
Chlorous acid, sodium salt (or sodium chlorite)	7758-19-2		X					X		
Choline Chloride	67-48-1		X			X	X	X	X	
Cinnamaldehyde	104-55-2	X	X		X	X	X	X	X	
Citric Acid	77-92-9	X	X		X	X	X	X	X	
Cocamidopropyl betaine	61789-40-0		X					X		
Cocoalkyl dimethylbenzyl ammonium chloride (ADBAC)	61789-71-7			X				X		
Coffee Extract	68916-18-7		X			X	X	X	X	
Cupric Nitrate	3251-23-8			X				X		
Dialuminium Chloride Pentahydroxide	12042-91-0			X				X		
Diammonium peroxidisulphate	7727-54-0		X			X	X	X	X	
Dichloromethane (methylene chloride)	75-09-2	X			X	X	X	X	X	
Diethanolamine	111-42-2		X			X	X	X	X	
Diethylene Glycol	111-46-6	X	X		X	X	X	X	X	
Diethylene glycol monobutyl ether	112-34-5	X			X	X	X	X	X	
Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane)	27306-78-1	X	X		X	X	X	X	X	
Disodium disulphite	7681-57-4			X		X	X	X	X	
Disodium metasilicate	6834-92-0	X			X	X	X	X	X	
Disodium octaborate tetrahydrate	12008-41-2	X	X		X	X	X	X	X	
Diutan	595585-15-2		X			X	X	X	X	
Diutan Gum	125005-87-0		X			X	X	X	X	
Ethanol	64-17-5		X			X	X	X	X	
Ethanol, 2,2'-oxybis-, reaction products with ammonia,morpholine derivatives residues	68909-77-3	X			X	X	X	X	X	
Ethoxylated alcohol	78330-21-9	X						X		
Ethyl hexanol	104-76-7	X						X		
Ethylene glycol	107-21-1		X			X	X	X	X	
Ethylene glycol monobutyl ether	111-76-2	X		X	X	X	X	X	X	
Ethylene oxide / propylene oxide copolymer	9082-00-2	X			X	X	X	X	X	
Ethylene oxide / propylene oxide copolymer	9003-11-6	X			X	X	X	X	X	
Fatty Acid Ester	10024-47-2	X			X	X	X	X	X	
Fatty Acids Ester	135800-37-2	X			X	X	X	X	X	
Fatty acids, tall-oil, ethoxylated	61791-00-2		X			X	X	X	X	
Food red 10	3734-67-6	X			X	X	X	X	X	
Formic Acid	64-18-6	X	X		X	X	X	X	X	
Gelatins	9000-70-8		X			X	X	X	X	
Glass, oxide	65997-17-3	X			X	X	X	X	X	
Glutaraldehyde	111-30-8		X	X				X		
Glycerine	56-81-5	X	X		X	X	X	X	X	
Glyoxal	107-22-2	X			X	X	X	X	X	
Graphite	7782-42-5	X			X	X	X	X	X	
Guar gum	9000-30-0		X			X	X	X	X	
Hemicellulase enzyme	9025-56-3		X			X	X	X	X	
Heterocyclic polymer containing nitrogen compounds	9003-39-8	X			X	X	X	X	X	
Hexamethylenediamine	124-09-4	X	X		X	X	X	X	X	
Hexamethylenetetramine	100-97-0	X			X	X	X	X	X	
Hexanedinitrile	111-69-3	X			X	X	X	X	X	
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	64742-47-8		X					X		
Hydrochloric Acid	7647-01-0		X	X				X		
Hydrogen Peroxide	7722-84-1			X				X		
Hydroxylpropyl guar	39421-75-5	X	X		X	X	X	X	X	

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Chemical Name	CAS No.	Assessed Activity(ies)			Assessed Use(s)					
		Drilling and Completions	Hydraulic Fracturing	Water Treatment	Residual Drilling Material	Irrigation	Stockwatering	Surface Water	Dust Supression/ Construction	TBA
Iron oxide	1309-37-1	X			X	X	X	X	X	
Isopropanol	67-63-0	X			X	X	X	X	X	
Isotridecanol, ethoxylated	69011-36-5	X						X		
Lactose	63-42-3		X			X	X	X	X	
Lecithins	8002-43-5	X			X	X	X	X	X	
Magnesium chloride	7786-30-3		X			X	X	X	X	
Magnesium nitrate	10377-60-3		X			X	X	X	X	
Magnesium oxide	1309-48-4	X			X	X	X	X	X	
Magnesium silicate hydrate (talc)	14807-96-6		X			X	X	X	X	
Melamine, formaldehyde, sodium bisulfite polymer	64787-97-9	X			X	X	X	X	X	
Methanol	67-56-1	X	X	X	X	X	X	X	X	
Methyl Acetate	79-20-9		X		X	X	X	X	X	
Mixture of dimer and trimer fatty acids of indefinite composition derived from tall oil	61790-12-3	X			X	X	X	X	X	
Modified bentonite	71011-24-0	X			X	X	X	X	X	
Monoethanolamine	141-43-5	X						X		
Monoethanolamine borate	26038-87-9		X			X	X	X	X	
N,N-Dimethylmethanamine	75-50-3		X			X	X	X	X	
Nitrilotriacetic acid, trisodium salt monohydrate	5064-31-3	X			X	X	X	X	X	
Nitrogen	7727-37-9	X	X		X	X	X	X	X	
Organic Derivative of Phosphonic Acid, K Salt	38820-59-6			X		X	X	X	X	
Oxazolidine	66204-44-2	X						X		
Peroxyacetic Acid	79-21-0			X				X		
Poly(vinyl acetate)-poly(vinyl alcohol) polymer	25213-24-5	X	X		X	X	X	X	X	
Polyalkylene Glycol Monobutyl Ether	9038-95-3	X			X	X	X	X	X	
PolyDADMAC	26062-79-3			X				X		
Polyethylene glycol	25322-68-3			X		X	X	X	X	
Polypropylene	9003-07-0	X			X	X	X	X	X	
Polypropylene Glycol	25322-69-4	X			X	X	X	X	X	
Polyquaternium-33	69418-26-4			X				X		
Polyurethane foam	9009-54-5	X			X	X	X	X	X	
Portland Cement	65997-15-1	X			X	X	X	X	X	
Potassium borate	1332-77-0		X			X	X	X	X	
Potassium Carbonate	584-08-7			X		X	X	X	X	
Potassium Chloride	7447-40-7	X	X		X	X	X	X	X	
Potassium Hydroxide	1310-58-3	X		X	X	X	X	X	X	
Potassium pyrophosphate	7320-34-5	X			X	X	X	X	X	
Potassium Sulphate	7778-80-5	X	X		X	X	X	X	X	
Silicic Acid, Potassium Salt	1312-76-1	X			X	X	X	X	X	
Silicon dioxide	112926-00-8		X		X	X	X	X	X	
Silicon dioxide	7631-86-9		X		X	X	X	X	X	
Silicon dioxide	112945-52-5		X		X	X	X	X	X	
Silicone based emulsion neutralised polyacrylic based stabiliser	NS	X			X	X	X	X	X	
Sodium Acetate	127-09-3		X		X	X	X	X	X	
Sodium Acid Pyrophosphate	7758-16-9	X			X	X	X	X	X	
Sodium Bicarbonate	144-55-8	X			X	X	X	X	X	
Sodium Bromide	7647-15-6			X		X	X	X	X	
Sodium Carbonate	497-19-8	X		X	X	X	X	X	X	
Sodium Carboxymethylcellulose	9004-32-4	X			X	X	X	X	X	
Sodium Chloride	7647-14-5	X			X	X	X	X	X	
Sodium Dodecyl Sulfate	151-21-3	X			X	X	X	X	X	
Sodium Erythorbate	6381-77-7	X			X	X	X	X	X	
Sodium gluconate	527-07-1		X			X	X	X	X	
Sodium Hydroxide	1310-73-2	X	X	X	X	X	X	X	X	
Sodium Hypochlorite	7681-52-9			X				X		
Sodium Iodide	7681-82-5		X		X	X	X	X	X	
Sodium lauryl polyoxyethylene ether sulfate	9004-82-4	X	X		X	X	X	X	X	
Sodium lignosulfonate	8061-51-6	X			X	X	X	X	X	
Sodium nitrite	7632-00-0	X			X	X	X	X	X	
Sodium persulfate	7775-27-1		X			X	X	X	X	
Sodium Polyacrylate	9003-04-7	X			X	X	X	X	X	
Sodium polynaphthalene sulfonate	9008-63-3	X			X	X	X	X	X	
Sodium silicate	1344-09-8	X			X	X	X	X	X	
Sodium Sulfate	7757-82-6		X			X	X	X	X	
Sodium sulphite	7757-83-7	X	X		X	X	X	X	X	
Sodium Tetraborate Decahydrate (Borax)	1303-96-4		X					X		
Sodium thiosulphate	7772-98-7	X	X		X	X	X	X	X	
Sorbitan monolaurate, ethoxylated	9005-64-5	X			X	X	X	X	X	
Sorbitan, mono-9-octadecenoate, (Z)	1338-43-8	X			X	X	X	X	X	
Sorbitan, mono-9-octadecenoate, ploy(oxy-1,2-ethanediyl) derivatives, (Z)	9005-65-6	X			X	X	X	X	X	
Soybean oil	8001-22-7	X			X	X	X	X	X	
Soybean oil, methyl ester, sulfated, sodium salt	68918-47-8	X			X	X	X	X	X	
Starch	9005-25-8	X			X	X	X	X	X	
Starch, carboxymethyl ether	9057-06-01	X			X	X	X	X	X	
Starch, polymer with (chloromethyl)oxirane	58944-89-1	X	X		X	X	X	X	X	
Sulfated oleic acid, potassium salt	68473-93-8	X			X	X	X	X	X	
Tetramethyl ammonium chloride	75-57-0		X			X	X	X	X	
Tributyl tetradecyl phosphonium chloride	81741-28-8		X					X		
Triethanolamine	102-71-6	X	X		X	X	X	X	X	
Trimethylamine hydrochloride	593-81-7		X			X	X	X	X	
Trisodium Citrate	68-04-2			X		X	X	X	X	
Ulexite	1319-33-1	X	X		X	X	X	X	X	
Vinylamide/vinyl sulfonated polymer	110897-64-8	X			X	X	X	X	X	
Vinylidene chloride/methylacrylate copolymer	25038-72-6		X			X	X	X	X	
Water (in Products)	7732-18-5	X	X		X	X	X	X	X	
Xanthan Gum	11138-66-2	X			X	X	X	X	X	
Silica										
Crystalline silica, cristobalite	14464-46-1	X			X	X	X	X	X	
Crystalline silica, quartz	14808-60-7	X			X	X	X	X	X	
Crystalline silica, tridymite	15468-32-3	X			X	X	X	X	X	
Diatomaceous earth	61790-53-2	X			X	X	X	X	X	
Non-crystalline silica (impurity)	7631-86-9		X			X	X	X	X	
Diatomaceous earth, calcined	91053-39-3		X			X	X	X	X	

Santos

Chemical Name	CAS No.	Assessed Activity(ies)			Assessed Use(s)					
		Drilling and Completions	Hydraulic Fracturing	Water Treatment	Residual Drilling Material	Irrigation	Stockwatering	Surface Water	Dust Supression/ Construction	TBA
Wood Products										
Almond Hulls	NS	X			X	X	X	X	X	
Nut Hulls	Mixture	X			X	X	X	X	X	
Vegetable Fibre	NS	X			X	X	X	X	X	
Walnut hulls	Mixture (1756)	X			X	X	X	X	X	
Wood fiber	Mixture (1757)	X			X	X	X	X	X	

Footnotes:

1 - Only required for new Tier 1 and Tier 2 chemicals

2 = PBT Assessment based on PBT Framework.

3 = Acute and chronic aquatic toxicity evaluated consistent with assessment criteria and framework.

4 = Categorisation as defined in assessment framework.

a - Similar polymers grouped together. See assessment for CAS NO.25085-02-3

b - Impurities present at de minimus levels. See assessment for CAS NO. 4080-31-3

c - Similar polymers grouped together. See assessment for CAS NO. 9003-11-6

d - Preponderance of data indicates appropriateness of Tier 2. See dossier for more information.

f - Similar polymers grouped together. See assessment for CAS NO. 25322-69-4

g - Preponderance of data indicates appropriateness of Tier 1. See dossier for more information.

h - Similar chemicals grouped together. See assessment for 14464-46-1/14808-60-7/15468-32-3/61790-53-2/7631-86-9/91053-39-3

i - Similar chemicals grouped together. Assessment for wood products includes almond hulls, nut hulls, walnut hulls, vegetable fibre a

k - Similar chemicals grouped together. See assessment for 595585-15-2/125005-87-0

Santos

Tier 1 Dossiers

Table of Contents

ACRYLAMIDE, SODIUM ACRYLATE POLYMER (CAS NO. 25987-30-8)
2-PROPENOIC ACID, POTASSIUM SALT, POLYMER WITH 2-PROPENAMIDE (CAS NO. 31212-13-2)
ACRYLATE TERPOLYMER (CAS NO. 903573-39-7)[1]
SILICONE BASED EMULSION NEUTRALISED POLYACRYLIC BASED STABILIZER (NO CAS NO.)

This group contains a sodium salt of a polymer consisting of acrylic acid, methacrylic acid or one of their simple esters and three similar polymers. They are expected to have similar environmental concerns and have consequently been assessed as a group. Information provided in this dossier is based on acrylamide/sodium acrylate copolymer (CAS No. 25085-02-3).

This dossier on acrylamide/sodium acrylate copolymer and similar polymers presents the most critical studies pertinent to the risk assessment of these polymers in their use in coal seam gas activities. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Acrylamide/sodium acrylate copolymer, acrylamide, sodium acrylate polymer and 2-propenoic acid, potassium salt, polymer with 2-propenamide are polymers of low concern. Therefore, these polymers and the other similar polymer in this group are classified as **tier 1** chemicals and require a hazard assessment only.

1. BACKGROUND

Acrylamide/sodium acrylate copolymer is a sodium salt of a polymer consisting of acrylic acid, methacrylic acid or one of their simple esters. Acrylates are a family of polymers which are a type of vinyl polymer. Synthetic chemicals used in the manufacture of plastics, paint formulations and other products. Acrylate copolymer is a general term for copolymers of two or more monomers consisting of acrylic acid, methacrylic acid or one of their simple esters.

Based largely on its high molecular weight, acrylamide/sodium acrylate copolymer are not expected to bioaccumulate or bioconcentrate. It is of low toxicity to environmental receptors and is not expected to degrade substantially under environmental conditions.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-Propenoic acid, sodium salt, polymer with 2-propenamide

CAS RN: 25085-02-3

Molecular formula: $(C_3H_5NO.C_3H_4O_2.NA)_x$-

Molecular weight: No information is available. Based on the type and intended use of the copolymer, the molecular weight would likely range from 100,000 to >3,000,000 g/mol (Hamilton *et al.*, 1997).

[1] CAS name: 2-Propenoic acid, polymer with sodium 2-hydroxy-3-(2-propen-1-yloxy)-1-propanesulfonate (1:1) and alpha-sulfo-omega-(2-propen-1-yloxy)poly(oxy-1,2-ethanediyl) ammonium salt (1:1), sodium salt

Synonyms: Acrylamide/sodium acrylate copolymer; 2-propenamide, polymer with 2-propenoic acid, sodium salt; 2-propenoic acid, sodium salt, polymer with 2-propenamide; 2-Propenamide-sodium 2 propenoate copolymer; sodium acrylate acrylamide polymer; sodium acrylate-acrylamide copolymer

3. PHYSICO-CHEMICAL PROPERTIES

No information is available.

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for acrylamide/sodium acrylate copolymer.

NICNAS has assessed acrylamide/sodium acrylate copolymer (CAS No. 25085-02-3), acrylamide, sodium acrylate polymer (CAS No. 25987-30-8) and 2-propenoic acid, potassium salt, polymer with 2-propenamide (CAS No. 31212-13-2) in an IMAP Tier 1 assessment and considers each a polymer of low concern[2].

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5. ENVIRONMENTAL FATE SUMMARY

No studies are available. The acrylamide/sodium acrylate copolymer is not expected to be readily biodegradable. The physico-chemical properties of the copolymer would preclude it from undergoing significant biodegradation (Guiney *et al.*, 1997). Biodegradation is limited due to the very high molecular weight and the low water solubility of the copolymer. The copolymer will likely bind tightly to organic matter found within soils and sediments (Guiney *et al.*, 1997). The copolymer is not expected to bioaccumulate because of its poor water solubility and high molecular weight.

6. ENVIRONMENTAL EFFECTS SUMMARY

No studies are available. Acrylamide/sodium acrylate copolymer is expected to be a low concern for toxicity to aquatic organisms (Guiney *et al.*, 1997). Due to its poor solubility and high molecular

[2] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.

weight, it is not expected to be bioavailable. It does not contain any reactive functional groups (*i.e.*, cationic groups).

7. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2017).

Acrylamide/sodium acrylate copolymer is not readily biodegradable; thus it meets the screening criteria for persistence.

Acrylamide/sodium acrylate copolymer is expected to have a very high molecular weight and poor water solubility. It is not expected to be bioavailable. Thus this copolymer does not meet the criteria for bioaccumulation.

There are no aquatic toxicity studies on acrylamide/sodium acrylate copolymer. It is expected to have low concern for aquatic toxicity because of its very high molecular weight and poor water solubility. Thus the copolymer does not meet the criteria for toxicity.

The overall conclusion is that acrylamide/sodium acrylate copolymer is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for acrylamide/sodium acrylate copolymer.

8. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Acrylamide/sodium acrylate copolymer	25085-02-3	Not a PBT	No	Yes	Yes	No	No	No	1	1	1
2-Propenoic acid, potassium salt, polymer with 2-propenamide	31212-13-2	Not a PBT	No	Yes	Yes	No	No	No	1	1	1
Acrylamide, sodium acrylate polymer	25987-30-8	Not a PBT	No	Yes	Yes	No	No	No	1	1	1
Acrylate Terpolymer	903573-39-7	Not a PBT	No	No	Yes	No	No	No	1	1	1
Silicone based emulsion neutralised polyacrylic based stabiliser	NS	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

NS = not supplied

CAS No. = chemical abstracts service number

COC = chemical of concern

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia. Available: http://www.nepc.gov.au/resource/chemical-risk-assessment-guidance-manuals

European Chemicals Agency (ECHA). (2017). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland. Available: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment

Guiney, P. D., McLaughlin, J. E., Hamilton, J. D., and Reinert, K. H. (1997). Dispersion Polymers. In: Ecological Assessment of Polymers Strategies for Product Stewardship and Regulatory Programs (Hamilton, J.D. and Sutcliffe, R. eds.), pp. 147-165, Van Nostrand Reinhold.

Hamilton, J. D., Vasconcellos, S. R., and Keener, R. L. (1997). Introduction. In: Ecological Assessment of Polymers Strategies for Product Stewardship and Regulatory Programs (Hamilton, J.D. and Sutcliffe, R. eds.), pp. 3-15, Van Nostrand Reinhold.

Klimisch, H. J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
CAS No.	Chemical Abstracts Service Number (also referred to as CAS RN)
COC	chemical of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IMAP	Inventory Multi-tiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

DISODIUM DISULPHITE

This dossier on disodium disulphite presents the most critical studies pertinent to the risk assessment of disodium disulphite in its use in coal seam gas activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Disodium disulphite is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Disodium disulphite is highly soluble in water and dissociates into sodium (Na^+), disulphite ($S_2O_5^{2-}$) ions and sulphur dioxide. Neither disodium disulphite nor its dissociated ions are expected to bioaccumulate. Disodium disulphite is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium disulphite

CAS RN: 7681-57-4

Molecular formula: $Na_2S_2O_5$

Molecular weight: 190.1 g/mol

Synonyms: Sodium metabisulphite, sodium pyrosulphite; sodium disulphite; disodium disulphite; sodium metabisulphite

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Disodium Disulphite

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White crystalline solid	2	ECHA
Melting Point	>150°C	2	ECHA
Density	2360 kg/m^3 @ 20 °C	2	ECHA
Water Solubility	667 g/L @ 25 °C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for disodium disulphite.

NICNAS has assessed sodium bromide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Disodium disulphite dissociates in aqueous media to sodium (Na^+) ions, disulphite ($S_2O_5^{2-}$) ions, and sulphur dioxide (SO_2). The disulphite ions can form bisulphite (HSO^{3-}) and sulphite ions (SO_2^{3-}) in varying proportions dependent on the pH of the solution (OECD, 2001).

Disodium disulphite is commonly used for removal of free chlorine. When dissolved in water, sodium bisulphite is formed from disodium disulphite:

$$Na_2S_2O_5 + H_2O \rightarrow 2\ NaHSO_3$$

and then reduces hypochlorous acid according to:

$$2\ NaHSO_3 + 2HOCl \rightarrow H_2SO_4 + 2\ HCl + Na_2SO_4$$

As an inorganic compound, biodegradation is not applicable to disodium disulphite. Disodium disulphite is not expected to bioaccumulate as it will dissociate to ions in aqueous solutions. Disodium disulphite is not expected to absorb to soil or sediment because of its dissociation properties and high water solubility.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7681-57-4%2C+

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No aquatic toxicity studies have been conducted on disodium disulphite. Other inorganic sulphite compounds show low-to-moderate toxicity concern to aquatic organisms. It is therefore expected that disodium disulphite is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

No acute aquatic studies were identified for disodium disulphite; however, studies were available on other inorganic sulphite compounds. The studies on these inorganic sulphite compounds can use to read-across to disodium disulphite since sulphite and bisulphite ions are formed in water upon dissociation of disodium disulphite. Table 3 lists the results of acute aquatic toxicity studies conducted on other inorganic sulphite compounds.

Table 3: Acute Aquatic Toxicity Studies on Inorganic Sulphite Compounds

Test Species	Endpoint	Results (mg/L)*	Klimisch score	Reference
Salmo gairdneri	96-hr LC_{50}	149.5	2	ECHA
Daphnia magna	48-hr EC_{50}	74.9	2	ECHA
Scenedesmus subspicatus	72-hr EC_{50} (Growth Rate)	36.8	2	ECHA

*mg $SO_3 2^-$/L

Chronic Studies

No chronic studies are available on disodium disulphite. However, studies are available on sodium sulphite. The studies on sodium sulphite can be used to read-across to disodium disulphite since sulphite and bisulphite ions are formed in water upon dissociation of disodium disulphite. Table 4 lists the results of chronic aquatic toxicity studies conducted on sodium sulphite.

Table 4: Chronic Aquatic Toxicity Studies on Sodium Sulphite (CAS No. 7757-83-7)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	NOEC	50	1	ECHA
Daphnia magna	21-d NOEC	>8.41	2	ECHA
Scenedesmus subspicatus	72-hr EC_{10}	28	2	ECHA

*mg SO_3^{2-}/L

C. Terrestrial Toxicity

No studies were identified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Disodium disulphite is an inorganic compound that dissociates completely to sodium ions, bisulphite and sulphite ions, and sulphur dioxide in aqueous solutions. Biodegradation is not applicable to these inorganic compounds. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to disodium disulphite or its dissociated compounds.

Disodium disulphite is an inorganic compound that dissociates completely in water to ionic species and gas. Thus, disodium disulphite is not expected to bioaccumulate.

There are no chronic aquatic toxicity studies on disodium disulphite. Disodium disulphite forms both bisulphite and sulphite ions upon dissociation in water. The NOECs from chronic aquatic toxicity studies on sodium sulphite are >0.1 mg/L. The acute E(L)C50 values for inorganic sulphite compounds are >1 mg/L in fish, invertebrates and algae. Thus, disodium disulphite does not meet the criteria for toxicity.

The overall conclusion is that disodium disulphite is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for disodium disulphite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Disodium disulphite	7681-57-4	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).
3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

OECD (2001). OECDS-SIDS: Disodium disulphite (CAS No. 7657-4). UNEP Publications. Available at: http://www.inchem.org/documents/sids/sids/DISODIUM.pdf

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

ORGANIC DERIVATIVE OF PHOSPHONIC ACID, K SALT

This dossier on organic derivative of phosphonic acid, K salt [also known as hexamethylenediamine tetra(methylenephosphonic acid), potassium salt (HMDTMP, K salt)] presents the most critical studies pertinent to the risk assessment of the chemical in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – HMDTMP, K salt is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

HMDTMP and its salts are phosphonic acid substances of very high water solubility, and low octanol-water partition coefficient. The phosphonic acid groups are multiply ionised at pH values relevant to biological and environmental systems. Ionisation gives them the ability to form stable complexes with metal ions, particularly polyvalent ones. Phosphonates are found to adsorb strongly to inorganic matrices, and hence they adsorb strongly to inorganic surfaces, soils and sediments, in model systems and mesocosms.

HMDTMP, K salt is not readily or inherently biodegradable. However, in the natural environment the fate and behaviour of HMDTMP and its ions are dominated by abiotic dissociation/complexing, irreversible adsorption to surfaces, more than by degradation processes (ECHA). If released to water, HMDTMP, K salt will partition primarily to water and suspended sediments. However, it has a low potential for bioaccumulation. HMDTMP, K salt is of low toxicity to aquatic organisms on an acute and chronic basis and of low toxicity to terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): potassium; [6-[bis[[hydroxy(oxido)phosphoryl]methyl]amino]hexyl-[[hydroxy(oxido)phosphoryl]methyl]amino]methyl-hydroxyphosphinate

CAS RN: 38820-59-6

Molecular formula: $C_{10}H_{28}N_2O_{12}P_4.x\text{-}K$

Molecular weight: 527.30 g/mol

Synonyms: Hexamethylenediamine tetra(methylenephosphonic acid), potassium salt; phosphonic acid, (1,6-hexanediylbis(nitrilobis(methylene)))tetrakis-, potassium salt; potassium;[6-[bis[[hydroxy(oxido)phosphoryl]methyl]amino]hexyl-[[hydroxy(oxido)phosphoryl]methyl]amino]methyl-hydroxyphosphinate

3 PHYSICO-CHEMICAL PROPERTIES

Limited chemical-specific information is available for HMDTMP, K salt. Key physical and chemical properties shown in Table 1 were obtained from the HMDTMP K salts group (EC RN 701-184-1).

Table 1 Overview of the Physico-chemical Properties of HMDTMP, K salt[1]

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid	-	ECHA
Melting Point	Will undergo decomposition when heating	1	ECHA
Boiling Point	Will undergo decomposition when boiling	-	ECHA
Density	1200 – 1300 kg/m^3 @ 20 °C	-	ECHA
Vapour Pressure	Negligible	2	ECHA
Partition Coefficient (log K_{ow})	-4.7	2	ECHA
Water Solubility	410 g/L @ 25 °C	-	ECHA
Dissociation constant (pKa)	1.3->10 @ 20 °C	2	ECHA

1 – Based on HMDTMP (4-7 K) (EC RN 701-184-1)

HMDTMP, K salt is freely soluble in water and, therefore, the HMDTMP anion is fully dissociated from its potassium cation (K^+) when in solution. The HMDTMP anion has eight P-OH groups that can be ionised. They lose a hydrogen to form a negatively charged group (P-O-). As the pH increases, the number of ionised groups increases. Under any given conditions, the degree of ionisation of the HDMTMP species is determined by the pH of the solution. Divalent and trivalent cations would preferentially replace the potassium ions. These would include calcium (Ca^{2+}), magnesium (Mg^{2+}) and iron (Fe^{3+}). These cations are more strongly bound by HMDTMP than potassium, forming stable complexes. (ECHA).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for HMDTMP, K salt.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No

Convention, Protocol or other international control	Listed Yes or No?
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

HMDTMP, K salt is a mineral-binding and complexing agent, with unusual chemical properties. HMDTMP and its salts adsorb strongly to inorganic surfaces, soils and sediments, in model systems and mesocosms, despite the very low log K_{ow} of -4.7. The nature of the adsorption is believed to be primarily due to interaction with inorganic substrate or generalised surface interactions. For example, the presence of calcium in solution tends to significantly increase the adsorption of similar phosphonate amino trimethylene phosphonic acid (ATMPA), similar effects are expected for HMDTMP. In natural waters this will play a part in the fate of HMDTMP, particularly in slightly alkaline waters, as this represents a route of abiotic removal from the environment (ECHA).

While some biodegradation has been observed, the results of aerobic and anaerobic biodegradation studies for HMDTMP and its salts do not show significant biodegradation in the short term, and they are not readily or inherently biodegradable. In reliable ready biodegradability studies, 0% degradation was observed in 28 days (ECHA) [Kl Score = 1].

Although biodegradation in soil has also not been demonstrated for HMDTMP and its salts, the role of abiotic removal processes is significant. There is no evidence for desorption occurring. Effectively irreversible binding is entirely consistent with the known behaviour of complexation and binding within crystal lattices. The high levels of adsorption which occur are therefore a form of removal from the environment; 5% remaining after 40 - 50 days is equivalent to a half-life of 10 days which is significant for the environmental exposure assessment (ECHA).

Based on these factors and that HMDTMP, K salt is hydrophilic, if released to water, HMDTMP and its salts will partition primarily to water and suspended sediments. However, given the very low measured value of log K_{ow} (-4.7), bioaccumulation is expected to be very low. No study of bioaccumulation conducted with HMDTMP or its salts is available. A reliable study of bioaccumulation of an analogous substance, DTPMP-7Na (CAS No. 22042-96-2) in *Cyprinus carpio*, indicates a BCF of <94 [Kl. Score = 1]. No active uptake mechanisms (i.e., mediated by enzymes) can occur for phosphonates (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

HMDTMP, K salt is of low toxicity concern for aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on HMDTMP, K salt.

Table 3 Acute Aquatic Toxicity Studies for HMDTMP, K Salt

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Salmo gairdneri (now known as Oncorhynchus mykiss) (Rainbow Trout)	72-hour LC_{50}	440	2	ECHA
Daphnia magna	48-hour EC_{50}	570	2	ECHA
Pseudokirchneriella subcapitatas	96-hour EC_{50}	28	2	ECHA

Chronic Studies

No long-term toxicity to fish or invertebrate data are available for HMDTMP or its salts. Toxicity data from read across to ATMPA (CAS No. 6419-19-8) are provided below in Table 4.

Table 4 Chronic Aquatic Studies on HMDTMP, K Salt[1]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykis (Rainbow Trout)	60-day NOEC	23	1	ECHA
Daphnia magna	28-day NOEC	≥25	2	ECHA

1-Toxicity data obtained from ATMPA (CAS No. 6419-19-8)

C. Terrestrial Toxicity

56-d NOEC and EC_{10} values of 556 and 543 mg active acid/kg soil dry weight have been determined for the effects of HMDTMP(4 -7K) on the reproduction of earthworms (*Eisenia fetida*) (ECHA). [Kl. Score = 1].

A 28-day EC_{50} value of >1000 mg active acid/kg soil dry weight has been determined for the effects of HMDTMP-(4-7K) on the nitrogen formation rate of soil microorganisms, based on nominal concentrations (ECHA) [Kl. Score = 1].

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

HMDTMP, K salt is not readily or inherently biodegradable. However, in the natural environment the fate and behaviour of HMDTMP and its ions are dominated by abiotic dissociation/complexing, irreversible adsorption to surfaces, more than by degradation processes (ECHA). Thus, HMDTMP, K salt does not meet the screening criteria for persistence.

The measured value of log K_{ow} (-4.7) is very low. Thus, HMDTMP, K salt does not meet the criteria for bioaccumulation.

The lowest NOEC from chronic aquatic toxicity studies is >0.1 mg/L. The acute EC_{50} values for HMDTMP, K salt are >1 mg/L in fish, invertebrates and algae. Thus, HMDTMP, K salt does not meet the screening criteria for toxicity.

The overall conclusion is that HMDTMP, K salt is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for the HMDTMP, K salt.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
HMDTMP, K salt	38820-59-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

POLYETHYLENE GLYCOL

This dossier on polyethylene glycol presents the most critical studies pertinent to the risk assessment of polyethylene glycol in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Polyethylene glycol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Polyethylene glycol is readily biodegradable, and it is not expected to bioaccumulate. It has low potential to adsorb to soil and sediment. Polyethylene glycol is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Poly(oxy-1,2-ethanediyl),α-hydro-ω-hydroxy- Ethane-1,2-diol, ethoxylated

CAS RN: 25322-68-3

Molecular formula: $C_{2n}H_{4n+2}O_{n+1}$

Molecular weight: variable (polymer)

Synonyms: Polyethylene glycol; poly(oxyethylene); polyethylene oxide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Polyethylene Glycol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Pale yellow organic liquid	1	ECHA
Melting Point	No freezing down to -14.08 °C @ 97.4 kPa	1	ECHA
Boiling Point	205.7°C @97.8 kPa	1	ECHA
Density	1,116 kg/m^3@ 20°C and 97.6 kPa	1	ECHA
Vapour Pressure	10 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	-0.698 @ 30°C and pH of 6.44	1	ECHA
Water Solubility	256 g/L at 25°C	1	ECHA
Viscosity	289.87 mPa s @20°C (dynamic)	1	ECHA

Polyethylene glycols are water-soluble linear polymers formed by the addition reaction of ethylene oxide to an ethylene glycol equivalent. The general formula for polyethylene glycol is: H-(OCH_2CH_2)$_n$-OH where “n” is the average number of repeating oxyethylene groups.

All of the lower molecular weight polyethylene glycols are liquid at room temperature; polyethylene glycols with higher molecular weights (defined as > 600 g/mol) exist as solids at room temperature.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for polyethylene glycol.

NICNAS has assessed polyethylene glycol in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Polyethylene glycol is readily biodegradable, and it is not expected to bioaccumulate. Polyethylene glycol has low potential to adsorb to soil and sediment.

[1]https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=25322-68-3

B. Biodegradation

Polyethylene glycol is readily biodegradable. In an OECD 301D test, there was 75% degradation after 28 days, as determined by oxygen consumption (ECHA) [Kl. score = 1]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

Experimental data are available for polyethylene glycol. In the key study, the soil organic carbon partition coefficient (K_{oc}) in soil and in sewage sludge of test chemical was determined by the Reverse Phase High Performance Liquid Chromatographic method according to OECD Guideline No. 121 for testing of Chemicals. The Log K_{oc} value of test chemical was determined to be 1.8568 dimensionless at 25°C (ECHA). [Kl. Score = 1].

Based upon this K_{oc} value, if released to soil, polyethylene glycol is expected to have low potential for adsorption and a high potential for mobility. If released to water, based on its K_{oc} and high water solubility values, polyethylene glycol is likely to remain in water and not adsorb to sediment. From the water surface, the substance will not evaporate into the atmosphere (ECHA).

D. Bioaccumulation

Using BCFBAF in EPISUITE™, the estimated the estimated BCF for polyethylene glycol is 3.162 L/Kg (ECHA). [Kl. Score = 2]. Based on this BCF value, the substance is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Polyethylene glycol is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on polyethylene glycol.

Table 3 Acute Aquatic Toxicity Studies on Polyethylene Glycol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Poecilia reticulata	96-hr LC_{50}	>100	2	ECHA
Daphnia magna	48-hour EC_{50}	>100	1	ECHA
Scenedesmus subspicatus	96-hour EC_{50}	>100	2	ECHA

Chronic Studies

Based on the EPISUITE™ ECOSAR version 1.11 predicted model, in 28 days long term fish toxicity (NOEC value) was estimated to be 13,671.586 mg/L on fish for on the basis of mortality effects (ECHA). [Kl. Score = 2].

The calculated value was further supported by 7-day freshwater study conducted on *Poecilia reticulata* (guppy fish) in semi-static conditions. The median lethal concentration of the test chemical (LC_{50}) was determined as 1150 mg/L (ECHA). [Kl. Score = 2].

Based on the EPISUITE™ ECOSAR version 1.10 predicted model, in 21 days long term aquatic invertebrate toxicity (NOEC value) was estimated to be 17,475.27 mg/L to Daphnid on the basis of reproductive effects (ECHA). [Kl. Score = 2].

Data for algae was available for read-across substance diethylene glycol mono-butyl ether (CAS No. 112-34-5). The effect of the test chemical to algae *Scenedesmus quadricauda* was performed for a period of 8 days. Based on the results obtained, the 8-day EC_{50} value was determined to be 1,000 mg/L (ECHA) [Kl. score = 2].

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Polyethylene glycol has been shown to be readily biodegradable; thus, it does not meet the screening criteria for persistence.

The calculated BCF is 3.162 L/kg. Thus, polyethylene glycol does not meet the screening criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on polyethylene glycol are >0.1 mg/L. The acute $E(L)C_{50}$ values from the acute aquatic toxicity studies on polyethylene glycol are >1 mg/L. Thus, polyethylene glycol does not meet the criteria for toxicity.

Therefore, polyethylene glycol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for polyethylene glycol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Polyethylene Glycol	25322-68-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = Bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

USEPA. (2016). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram

LC	lethal concentration
mg	milligrams
mg/L	milligrams per litre
NICAS	National Industrial Chemicals Notification and Assessment Scheme
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

POTASSIUM CARBONATE

This dossier on potassium carbonate does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies pertinent to the risk assessment of potassium carbonate in its use in coal seam gas activities. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Potassium carbonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Potassium carbonate is soluble in water, dissociating into potassium (K^+) and carbonate (CO_3^{2-}) ions. Both ions are ubiquitous in the environment. Biodegradation is not applicable to these inorganic ions. Potassium carbonate does not bioaccumulate and is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Dipotassium carbonate

CAS RN: 584-08-7

Molecular formula: K_2CO_3

Molecular weight: 138.21 g/mol

Synonyms: Dipotassium carbonate; potassium carbonate; potash; salt of tartar; carbonic acid, potassium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Potassium Carbonate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Hydroscopic white powder or crystals	2	ECHA
Melting Point	891°C @ 101.3 kPa	2	ECHA
Boiling Point	Not determined due to decomposition.	2	ECHA
Density	2,430 kg/m^3 @ 19°C	2	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	ca. 1,100 g/L @ 20°C	2	ECHA
Dissociation constant (pKa)	6.35 and 10.33 @ 25 °C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for potassium carbonate.

NICNAS has assessed potassium carbonate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Potassium carbonate is soluble in water, dissociating into potassium (K^+) and carbonate (CO_3^{2-}) ions. Both ions are ubiquitous in the environment.

The addition of potassium carbonate to an aquatic ecosystem could result in a shift towards alkalinity and a tendency to increase the pH. The carbonate ions will react with water, forming bicarbonate (HCO_3^-) and hydroxide (OH^-) ions, until an equilibrium is reached. A re-equilibration takes place when carbonate (CO_3^{2-}) is dissolved in water according to the following equations:

$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ $pK_a = 10.33$

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ $pK_a = 6.35$

[1]https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=584-08-7

Only a small fraction of the dissolved CO_2 is present as H_2CO_3 (carbonic acid); the major part is present as CO_2. The amount of CO_2 in water is in equilibrium with the partial pressure of CO_2 in the atmosphere. The $CO_2/HCO_3^-/CO_3^{2-}$ equilibria are the major buffer of the pH of freshwater.

Based on these equations, CO_2 is the predominant species at a pH smaller than 6.35, while HCO_3^- is the predominant species at a pH in the range of 6.35-10.33 and CO_3^{2-} is the predominant species at a pH higher than 10.33.

K^+ and CO_3^{2-} ions are not expected to adsorb on particulate matter or surfaces and will not bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Potassium carbonate is of low acute toxicity concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on potassium carbonate.

Table 3 Acute Aquatic Toxicity Studies on Potassium Carbonate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hr LC_{50}	68	2	ECHA
Lepomis macrochirus	96-hr LC_{50}	230	2	ECHA
Daphnia pulex	48-hr EC_{50}	200	2	ECHA
Daphnia magna	48-hr EC_{50}	430	2	ECHA

No data was available for algae. Potassium carbonate is not expected to have an intrinsic toxic activity to aquatic plants (ECHA).

Chronic Studies

No studies are available. Potassium carbonate is not expected to have an intrinsic toxic activity to aquatic organisms (ECHA).

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium carbonate is an inorganic salt that dissociates completely to potassium and carbonate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both potassium and carbonate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Potassium and carbonate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Thus, potassium carbonate is not expected to bioaccumulate.

No chronic aquatic toxicity data exist on potassium carbonate; however, the acute E(L)C_{50} values are >1 mg/L in fish and invertebrates. Thus, potassium carbonate does not meet the screening criteria for toxicity.

The overall conclusion is that potassium carbonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium carbonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Potassium Carbonate	584-08-7	Not a PBT	No	No	NA	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SODIUM BROMIDE

This dossier on sodium bromide presents the most critical studies pertinent to the risk assessment of sodium bromide in its use in coal seam gas activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium bromide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium bromide is an inorganic salt and is highly soluble. Sodium bromide is expected to be fully dissociated to sodium and bromide ions in water and therefore is unlikely to adsorb to soil or sediment. Biodegradation is not applicable to these inorganic ions. Sodium bromide does not bioaccumulate and is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium bromide

CAS RN: 7647-15-6

Molecular formula: NaBr

Molecular weight: 102.89 g/mol

Synonyms: Bromide salt of sodium

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Bromide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White or colourless crystalline solid	2	ECHA
Melting Point	755°C @ 101.3 kPa	2	ECHA
Boiling Point	1,390°C @ 101.3 kPa	-	ECHA
Density	3,210 kg/m^3 @ 20°C	2	ECHA
Water Solubility	946 g/L @ 25 °C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium bromide.

NICNAS has assessed sodium bromide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium bromide is an inorganic salt that is highly soluble in water and is expected to fully dissociate to sodium and bromide ions in water, and therefore is unlikely to adsorb to soil or sediment. Biodegradation is not applicable to these inorganic ions.

B. Partitioning

Bromide ions would be expected to partition to water rather than soils and sediments in the environment given their high water solubility (ca. 90 g per 100 mL for sodium bromide) and the negative charges on the ions available (ECHA)

C. Biodegradation

Sodium bromide dissociates in aqueous solutions to sodium (Na^+) and bromide (Br^-) ions. Biodegradation is not applicable to these inorganic ions.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7647-15-6

D. Environmental Distribution

Bromide ions would be expected to partition to water rather than soils and sediments, therefore the organic carbon partition coefficient (K_{oc}) is assumed to be very low (ECHA). The mobility of bromide ions in soils is therefore assumed to be very high.

E. Bioaccumulation

Sodium bromide is not expected to bioaccumulate.

As noted above, sodium bromide dissociates in aqueous solution to the metal ion (Na^+) and bromide ions (Br^-). The bioaccumulation of sodium bromide in aquatic invertebrates (*Artemia salina larvae*) was determined using a concentration of 10% LC_{50} of the test substance (53.11 mg/L) (ECHA). An estimated bioconcentration factor for sodium bromide was 0.23 (ECHA) [Kl. Score = 2] and, as such, concluded that sodium bromide poses no bioaccumulation risk to aquatic invertebrates.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium bromide is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sodium bromide.

Table 3 Acute Aquatic Toxicity Studies on Sodium Bromide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Scophthalmus maximus	96-hr LC_{50}	>440	2	ECHA
Daphnia magna	48-hr LC_{50}	>1,000	2	ECHA
Lemna minor	NOEC	3,200	2	ECHA

Chronic Studies

A reproductive toxicity test with sodium bromide on male and female fish (*Poecilia reticulata*) was performed and the No Observed Effect Concentration (NOEC) based on reproduction was determined to be 10 mg/L (ECHA). [Kl. Score = 2].

The 16d-NOEC of sodium bromide on *Daphnia magna was* determined to be 2.8 mg/L based on observation criteria of growth effects (ECHA). [Kl. Score = 2].

C. Terrestrial Toxicity

The acute toxicity of sodium bromide to the earthworm (*Eisenia foetida*) showed the NOEC was 10 mg bromide/kg on the basis that no mortalities were observed after 14 days exposure and additionally no sub-lethal effects on weight or behaviour were observed at 10 mg bromide/kg. The short-term EC_{50} or LC_{50} for soil microorganisms was estimated to be 1,000 mg/kg soil dry weight (ECHA). [Kl. Score = 1].

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium bromide is an inorganic salt that dissociates in aqueous solutions to sodium (Na^+) and bromide (Br^-) ions. Biodegradation is not applicable to these inorganic ions, thus it does not meet the screening criteria for persistence.

Sodium bromide is an inorganic salt and is not expected to bioaccumulate and therefore does not meet the screening criteria for bioaccumulation.

The lowest NOEC value on sodium bromide is >0.1 mg/L for invertebrates and fish. The acute $E(L)C_{50}$ values are >1 mg/L in fish, invertebrates and algae. Thus, sodium bromide does not meet the screening criteria for toxicity.

The overall conclusion is that sodium bromide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium bromide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Bromide	7647-15-6	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = Bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg	milligrams
mg/L	milligrams per litre

NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observable effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

TRISODIUM CITRATE

This dossier on trisodium citrate presents the most critical studies pertinent to the risk assessment of trisodium citrate in its use in coal seam gas activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on citric acid (OECD 2001a,b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Trisodium citrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Trisodium citrate is readily biodegradable and is not expected to bioaccumulate. Trisodium citrate is the sodium salt of citric acid. This compound can be referred to as simply sodium citrate, though sodium citrate can refer to any of the three trisodium salts of citric acid (namely trisodium citrate, trisodium citrate dihydrate and trisodium citrate pentahydrate). Trisodium citrate is highly soluble and is expected to be fully dissociated to citrate and sodium ions in water and therefore is unlikely to adsorb to soil or sediment. Trisodium citrate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Trisodium 2-hydroxypropane-1,2,3-tricarboxylate

CAS RN: 68-04-2

Molecular formula: $C_6H_8Na_3O_7$

Molecular weight: 258.06 g/mol

Synonyms: Sodium citrate; trisodium 2-hydroxypropane-1,2,3-tricarboxylate; 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, trisodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Trisodium Citrate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Crystalline solid	2	ECHA
Melting Point	>150°C (pressure not reported)	2	ECHA
Boiling Point	Not available; decomposition	-	ECHA
Density	1,857 kg/m^3 @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	Negligible @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	-0.2 to -1.8 for citric acid (temperature not provided)	4	ECHA
Water Solubility	@ 400 – 700 g/L @ 20-25 °C	4	ECHA
Dissociation constant (pKa)	3.13, 4.76, 6.4 @ 25 °C for citric acid	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for trisodium citrate.

NICNAS has assessed trisodium citrate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Trisodium citrate is readily biodegradable. It is not expected to bioaccumulate. Trisodium citrate is highly soluble and is expected to be fully dissociated to citric acid/citrate and sodium ions in water and therefore is unlikely to adsorb to soil or sediment.

B. Partitioning

Trisodium citrate lacks any of the functional group that are susceptible to hydrolysis in aqueous solution.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=68-04-2

C. Biodegradation

Trisodium citrate dissociates in aqueous solutions to sodium (Na^+) and citrate ($C_6H_5O_7^-$) ions. Trisodium citrate can be considered readily biodegradable based on the results of the ready and inherent aerobic biodegradation studies on citric acid/citrate listed in Table 3.

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

Table 3 Biodegradation Studies on Citric Acid (OECD 2001a,b)

Test System	Results*	Notes	Klimisch Score
Modified Sturm	97% (CO_2 evolution); 100% (DOC removal)	Readily biodegradable; exposure period not stated	2
Closed Bottle Test	BOD_{30}/COD Ratio = 90%	Readily biodegradable	2
BOD_5/COD Ratio	BOD_5 = 526 mg; COD = 728 mg; BOD_5/COD Ratio = 0.72	Readily biodegradable; concentration of test substance and activated sludge not stated	2
BOD_1/ThOD Ratio	BOD_1/ThOD Ratio = 13%	-	2
BOD_{20}/ThOD Ratio	BOD_{20}/COD Ratio = 98%	Readily biodegradable; initial test substance concentration 720 mg/L	2
Zahn-Wallen Test	85%, 1 day (DOC removal)	Inherently biodegradable	2
Zahn-Wallen Test	98%, 7 days (DOC removal)	Inherently biodegradable	
Coupled Units Test	93% (COD removal)	Ultimately biodegradable; exposure period not stated	2

D. Environmental Distribution

No experimental data are available for trisodium citrate or citric acid. Using KOCWIN program in EPISuite™ (USEPA, 2016), the estimated soil organic carbon partition coefficient (K_{oc}) value for citric acid from the octanol/water partition coefficient (K_{ow}) value of -1.08 is 0.3617 L/kg.

If released to soil, based on this negligible K_{oc} value, this substance is unlikely to adsorb to soil and would be highly mobile. If released to water, based on a negative K_{ow} value and high water solubility, this substance is unlikely to adsorb to suspended solids and would preferentially partition to the water column.

E. Bioaccumulation

The log K_{ow} for trisodium citrate is very low and falls between -0.2 to -1.8. Thus, trisodium citrate is not expected to bioaccumulate.

As noted above, trisodium citrate dissociates in aqueous solution to the metal ion (Na^+) and citrate ions ($H_7C_6O_7^-$). Citrate is found in all eukaryotic cells as an intermediate of the Tricarboxylic acid (TCA)

cycle, which is part of the basic metabolic pathway that generates useable energy from carbohydrates, proteins and fats. Citric acid is formed and broken down in the course of this cycle at very high rates (ECHA).

An estimated BCF for citric acid was 3.2 L/kg (ECHA) [Kl. Score = 2]. The weight of evidence of the low estimated BCF, biodegradability and role in cell metabolism indicate that citric acid is extremely unlikely to bioaccumulate (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Trisodium citrate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

No reliable data is available assessing the toxicity of trisodium citrate to fish or algae, however, data for the parent compound, citric acid, is available. Table 4 lists the results of acute aquatic toxicity studies conducted on citric acid (CAS No. 77-92-9).

Table 4 Acute Aquatic Toxicity Studies on Trisodium Citrate*

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Leuciscus idus melanotus (golden orfe)	48-hr LC_{50}	590	2	ECHA
Daphnia magna	48-hr EC_{50}	2,055	2	ECHA

*Value based on citric acid converted to trisodium citrate using a factor of 1.34 (ECHA)

In addition, the 8-day toxicity threshold value (EC_0) for citric acid in *Scenedesmus quadricauda* is 640 mg/L, from which a NOEC value of 425 mg/L (citric acid) was derived. However the algal study should not be considered due to the essential nutrient complexing properties of the test substance that do not permit to assess the true toxicity of the test substance (ECHA). [Kl. Score = 2].

Chronic Studies

No studies are available. As outlined in ECHA, testing is not considered necessary because:

- Short-term toxicity to aquatic organisms is low.
- Risk characterisation ratios based on $PNEC_{aquatic}$ calculated using the short-term data are <1.
- The parent acid substance is naturally occurring in aquatic organisms and so is the counter ion.

C. Terrestrial Toxicity

No studies are available. The substance has a negative log K_{ow} value and therefore, partitioning to the terrestrial compartment is expected to be minimal (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Trisodium citrate is readily or inherently biodegradable; thus, it does not meet the screening criteria for persistence.

The log K_{ow} values for trisodium citrate is between -0.2 and -1.8. Thus, trisodium citrate does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on citric acid or trisodium citrate. The acute E(L)C_{50} values for citric acid are >1 mg/L in fish and invertebrates. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that trisodium citrate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for trisodium citrate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Trisodium Citrate	68-04-2	Not a PBT	No	No	No	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

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USEPA. (2016). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
COD	chemical oxygen demand
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union

g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg	milligrams
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TCA	tricarboxylic acid
ThOD	theoretical oxygen demand
USEPA	United States Environmental Protection Agency

SORBITAN, MONO-9-OCTADECENOATE, (Z)

This dossier on sorbitan, mono-9-octadecenoate, (Z) presents the most critical studies pertinent to the risk assessment of sorbitan, mono-9-octadecenoate, (Z) in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sorbitan, mono-9-octadecenoate, (Z) is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sorbitan mono-9-octadecenate, (Z) is a hydrophilic, non-ionic surfactant used as an emulsifier. Sorbitan mono-9-octadecenate, (Z) is readily biodegradable and not expected to persist in the environment, and due to expected metabolism is not likely to bioaccumulate. Acute and chronic studies indicate that the substance is of relatively low toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): [(2*R*)-2-[(2*R*,3*R*,4*S*)-3,4-dihydroxyoxolan-2-yl]-2-hydroxyethyl] (*Z*)-octadec-9-enoate

CAS RN: 1338-43-8

Molecular formula: $C_{24}H_{44}O_6$

Molecular weight: 428 g/mol

Synonyms: Sorbitan monooleate; sorbitan, mono-9-octadecenoate, (Z)

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for sorbitan, mono-9-octadecenoate, (Z) are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sorbitan mono-9-octadecenate, (Z)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Yellow to amber liquid		HPVIS
Melting point	223 °C (estimated, pressure not provided)		HPVIS
Boiling point	535 °C (estimated, pressure not provided)		HPVIS

Property	Value	Klimisch score	Reference
Density	1000 kg/m^3 @ 25°C		HPVIS
Vapour pressure	Negligible		HPVIS
Partition coefficient (log K_{ow})	5.89 (estimated), temperature not provided		HPVIS
Water solubility	0.0191 (estimated) (insoluble) @ 25°C		PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sorbitan, mono-9-octadecenoate, (Z).

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Environmental fate data of the substance or reasonable surrogates suggests that it will degrade in the environment, not persist, and due to expected metabolism is not likely to bioaccumulate.

The data supporting these conclusions are discussed below.

B. Biodegradation

Sorbitan, mono-9-octadecenoate, (Z) is readily biodegradable. In an OECD 301 C test, degradation was 58% after 14 days and 62% after 28 days (HPVIS). In a read-across, sorbitan stearate (CAS No. 1338-41-6) is readily biodegradable. In an OECD 301 C test, degradation was 88% after 28 days (ECHA) [Kl. score = 1].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for sorbitan, mono-9-octadecenoate, (Z). Using KOCWIN in EPISUITE™ (U.S. EPA, 2019), the estimated K_{oc} value from log K_{ow} is 1,599 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 2,423 L/kg. Based on these estimated K_{oc} values, the substance is likely to adsorb to soil or sediments, and unlike other more immobile Sorbitan Esters in this category, will have slight mobility.

D. Bioaccumulation

There are no bioaccumulation studies on sorbitan, mono-9-octadecenoate, (Z). Sorbitan, mono-9-octadecenoate, (Z) has an estimated log K_{ow} of 5.89 (U.S. EPA, 2019). However, sorbitan, mono-9-octadecenoate, (Z) is expected to be metabolised and excreted. The metabolic pathway involves enzymatic hydrolysis by esterases to D-glucitol and the respective fatty acid. The fatty acids are metabolised by the beta-oxidation pathway and D-glucitol will undergo metabolism by the fructose metabolic pathway in the liver (ECHA). Using the Arnot-Gobas method involving biotransformation in the QSAR model BCFBAF v3.01, the BCF values ranged from 36 to 92 L/kg, indicating a low potential for bioaccumulation (U.S. EPA, 2019).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Acute and chronic studies indicate that the substance is of relatively low toxicity to aquatic organisms. Data to support this conclusion are discussed below.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sorbitan, mono-9-octadecenoate, (Z) or sorbitan stearate.

Table 3 Acute Aquatic Toxicity Studies on Sorbitan, Mono-9-octadecenoate, (Z) and Sorbitan Stearate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Salmo gairdneri	96-hr LL_{50}	>1,000 [WAF]	2	HPVIS
Oryzias latipes	96-hr LL_{50}	>1,000 [WAF]*	1	ECHA
Daphnia magna	48-hr EL_{50}	>1,000 [WAF]*	1	ECHA
Pseudokirchneriella subcapitata	72-hr EL_{50}	>1,000 [WAF]*	1	ECHA

*Studies conducted on sorbitan stearate (CAS No. 1338-41-6).

Chronic Studies

The 21-day NOELR (no-observed-effect-loading-rate) in a *Daphnia* reproduction test for sorbitan stearate (CAS No. 1338-41-6) is 16 mg/L WAF (ECHA) [Kl. score = 2].

The 72-hr NOELR (no-observed-effect-loading-rate) to *Pseudokirschneriella subcapitata* for sorbitan stearate is 560 mg/L (WAF) (ECHA) [Kl. score = 1].

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sorbitan, mono-9-octadecenoate, (Z) is not readily biodegradable; however, it is expected to be inherently biodegradable; thus, it does not meet the screening criteria for persistence.

The estimated BCF values (involving biotransformation) for sorbitan, mono-9-octadecenoate, (Z) ranged from 36 to 92 L/kg. Thus, it does not meet the criteria for bioaccumulation.

The lowest chronic NOELR for sorbitan stearate, the surrogate for sorbitan, mono-9-octadecenoate, (Z), is >0.1 mg/L. The acute EL_{50} values are >1 mg/L. Thus, sorbitan, mono-9-octadecenoate, (Z) does not meet the screening criteria for toxicity.

The overall conclusion is that sorbitan, mono-9-octadecenoate, (Z) is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sorbitan, mono-9-octadecenoate, (Z).

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sorbitan, mono-9-octadecenoate, (Z)	1338-43-8	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EL	Effective Limit
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry

kg	kilogram
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
LL	Lower limit
MCI	molecular connectivity index
mg/L	milligrams per litre
NOELR	no-observed-effect-loading-rate
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
WAF	Water accommodated fraction

CASTOR OIL

This dossier on castor oil presents the most critical studies pertinent to the risk assessment of this substance in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the data published in the ECHA dossier for Castor Oil Dehydrated (CAS No. 64147-40-6) (ECHA, 2020). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Castor oil is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Castor oil is extracted from the Ricinus communis seeds plant. Like other vegetable oils, castor oil is a triacylglycerol composed of various fatty acids and glycerol. Castor oil is expected to be broken down by a range of microorganisms; and, therefore, is not expected to persist or bioaccumulate. In general, castor oil is of relatively low aquatic toxicity.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Castor Oil

CAS RN: 8001-79-4

Molecular formula: $C_{57}H_{104}O_9$ (Computed by PubChem 2.1 (PubChem release 2019.06.18))

Molecular weight: 933.4 g/mol (Computed by PubChem 2.1 (PubChem release 2019.06.18)

Synonyms: 2,3-bis[[(Z)-12-hydroxyoctadec-9-enoyl]oxy]propyl (Z)-12-hydroxyoctadec-9-enoate; Ricinus oil; Olio di ricino; Venelex; Xenaderm; Optase

3 PHYSICO-CHEMICAL PROPERTIES

Specific physico-chemical properties on castor oil are unavailable. Therefore, data from a similar substance, dehydrated castor oil (CAS No. 8001-79-4), are presented in Table 1.

Table 1 Overview of the Physico-chemical Properties of Castor Oil Dehydrated (CAS No. 64147-40-6)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Pale-yellow or almost colorless transparent viscous liquid	-	ECHA
Melting/Freezing point	< -34°C (pressure not provided)	1	ECHA
Boiling point	366°C @ 101.3 kPa	1	ECHA
Vapour pressure	0 Pa @ 20°C	1	ECHA

Property	Value	Klimisch score	Reference
Density	950 kg/m^3 @ 20°C	1	ECHA
Partition coefficient (log K_{ow})	>16 (QSAR)	2	ECHA
Water solubility	0.005 g/L @ 20°C (insoluble)	1	ECHA
Viscosity	607 mPa s @ @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for castor oil.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Specific environmental fate properties on castor oil are unavailable. Therefore, data from a similar substance, dehydrated castor oil (CAS No. 64147-40-6), are presented below. The substance is expected to adsorb but not persist or bioaccumulate. Specific data are discussed below.

B. Biodegradation

A study was conducted to determine the ready biodegradability of castor oil, dehydrated according to EC Method C.4-D and OECD Guideline 301 F (manometric respirometry test) [Kl. score = 1].

Biodegradation was followed via oxygen uptake of microorganims from non-adapted domestic sludge over a period of 28 days.

Under the test conditions, the degradation rate of the test substance did not reach 60% within the 10-day window and after 28 days of incubation.

Overall, these substances (i.e. triglycerides and adducts thereof) are well known to be easily broken down by a range of microorganisms such as gram-positive or gram-negative bacteria, a number of fungi and yeasts as well as several types of algae, regardless of their functional groups and chain length (ECHA, 2020). Therefore, while they do not meet the stringent criteria for classification as readily biodegradable and have modelled half-lives in soil of up to 120 days, they do biodegrade and thus castor oil, dehydrated is not expected to persist in the aquatic or soil environment.

C. Environmental Distribution

The estimated soil adsorption coefficients (log K_{oc}) of C18:0 triglyceride and the adduct formed by two C18:3 triglycerides using KOCWIN v.2.00 (EPIWEB v.4.1) were found to be ca. 14 and 25, respectively [Kl. score = 2].

When released to the environment, castor oil, dehydrated, based on low water solubility and log K_{oc} values greater than 14, is likely to partition to soil and sediment and be immobile. However, as detailed in the following Section, here it is expected to be broken down by a range of microorganisms and not persist.

D. Bioaccumulation

The bioaccumulation potential as indicated by its bioconcentration factor (BCF) of castor oil, dehydrated was estimated according to the BCFBAF v.3.01 model of EPIWEB v.4.1 considering a range of components present in the substance, i.e. from a C18:0 triglyceride to an adduct formed by two C18:3 triglycerides (ECHA, 2020). The BCF was equivalent to 3.162 L/kg wet weight in all cases, which corresponds to a low bioaccumulation potential [Kl. score = 2].

Based on low water solubility and high adsorption coefficient, the substance is unlikely to be significantly bioavailable to aquatic organisms. When ingested, the constituent triglycerides are well known to be broken down into glycerol and fatty acids which then undergo β-oxidation and are used as a source of energy (ECHA, 2020). As such, castor oil, dehydrated is not expected to bioaccumulate in aquatic organisms.

6 ENVIRONMENTAL EFFECT SUMMARY

A. Summary

Acute and chronic aquatic toxicity studies were performed on a variety of species/trophic levels with algae exhibiting greater sensitivity to the substance. In general, the substance is of relatively low aquatic toxicity. Study results are presented below.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 lists the results of acute aquatic toxicity studies conducted on the subject substance.

Table 3 Acute Aquatic Toxicity Studies on Castor Oil Dehydrated (CAS No. 64147-40-6)

Guideline/Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
OECD Guideline 203/ *Brachydanio rerio*	96-hr LC_{50}	>100	2	ECHA, 2020
OECD Guideline 202/ *Daphnia magna*	48-hr EC_{50}	>100	2	ECHA, 2020
OECD Guideline 201/ *Pseudokirchneriella subcapitata*	72-hr EC_{50}	>100	2	ECHA, 2020

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Persistence: Under the test conditions, the degradation rate of the test substance did not reach 60% within the 10-day window and after 28 days of incubation. However, these substances (i.e. triglycerides and adducts thereof) are well known to be easily broken down by a range of microorganisms such as gram-positive or gram-negative bacteria, a number of fungi and yeasts as well as several types of algae, regardless of their functional groups and chain length. Therefore, while they do not meet the stringent criteria for classification as readily biodegradable and have modelled half-lives in soil of up to 120 days, they do biodegrade and thus castor oil, dehydrated is not expected to persist in the aquatic or soil environment.

Bioaccumulation: The bioconcentration factor (BCF) of castor oil, dehydrated was estimated according to the BCFBAF v.3.01 model of EPIWEB v.4.1 considering a range of components present in the substance, i.e. from a C18:0 triglyceride to an adduct formed by two C18:3 triglycerides. The BCF was equivalent to 3.162 L/kg wet weight (log BCF = 0.5) in all cases, which corresponds to a low bioaccumulation potential.

Toxicity: The lowest NOEC values from acute aquatic toxicity studies on fish, invertebrates and algae are all >100 mg/L. Thus, the substance is not considered toxic according to the specified criteria.

The overall conclusion is that castor oil is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for castor oil.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Castor oil	8001-79-4	Not a PBT	No	No	No	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

DEWHA. 2009. Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts (DEWHA), Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

ECHA. 2008. Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency (ECHA), Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCFBAF™	program module of EPAWEB v4.1 to estimate fish bioconcentration factor and its logarithm
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
KOCWIN™	program module of EPIWEB v4.1 to estimate the organic carbon-normalized sorption coefficient for soil and sediment
kPa	kilopascal
L	litre
LC	lethal concentration
mg/L	milligrams per litre
mPa s	millipascal - second

NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SORBITAN, MONODODECANOATE, POLY (OXY-1,2-DIETHANEDIYL)

This dossier on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) presents the most critical studies pertinent to the risk assessment of sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is a hydrophilic, non-ionic surfactant used as an emulsifier. It is considered a UVCB substance (substance of unknown or variable composition, complex reaction products or biological materials). Based on the substance group types evaluated, the substance is readily biodegradable; has a low potential for bioaccumulation; and a high potential for adsorption to soil and sediment. It is of low-to-moderate toxicity concern to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sorbitan monolaurate, ethoxylated

CAS RN: 9005-64-5

Molecular formula: Not available (UVCB substance)

Molecular weight: Not available (UVCB substance)

Synonyms: See below.

The composition of sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) (CAS No. 9005-64-5) is unknown. The CAS No. 9005-64-5 is a generic CAS No. that can include at least the following UVCB substance groups:

1. A mixture of laurate esters of sorbitol and sorbitol anhydrides, consisting predominantly of the monoester, condensed with approximately 4 moles of ethylene oxide (e.g., Polysorbate 21).

2. An ethoxylated sorbitan ester of lauric acid with an average of 10 moles of ethylene oxide (e.g., PEG-10 sorbitan laurate).

3. A mixture of laurate esters of sorbitol and sorbitol anhydrides, consisting predominantly of the monoester, condensed with approximately 20 moles of ethylene oxide (e.g., Polysorbate 20).

4. An ethoxylated sorbitan ester of lauric acid with an average of 40 moles of ethylene oxide (e.g., PEG-40 sorbitan laurate).

5. An ethoxylated sorbitan ester of lauric acid with an average of 44 moles of ethylene oxide (e.g., PEG-44 sorbitan laurate).

6. An ethoxylated sorbitan ester of lauric acid with an average of 75 moles of ethylene oxide (e.g., PEG-75 sorbitan laurate).

7. An ethoxylated sorbitan ester of lauric acid with an average of 80 moles of ethylene oxide (e.g., PEG-80 sorbitan laurate).

This dossier will include information from the following substances:

Polysorbate 20 (CAS No. 9005-64-5)

Sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5]

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sorbitan Monolaurate, Ethoxylated (1 - 6.5 Moles Ethoxylated) (CAS No. 9005-64-5)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Lemon- to amber-coloured oily liquid	2	ECHA
Melting point	-64 to -22°C @ 101.3 kPa	2	ECHA
Boiling point	-	-	-
Density	1095 kg/m^3 @ 20°C	2	ECHA
Vapour pressure	Negligible	2	ECHA
Partition coefficient (log K_{ow})	1.23 to 3.86 (QSAR)	2	ECHA
Water solubility	<0.0002 g/L @ 20°C	1	ECHA
Dissociation constant (pKa)	13.84 – 13.89 @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns

were identified within Australia and internationally for sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl).

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is readily biodegradable; has a low potential for bioaccumulation; and a high potential for adsorption to soil and sediment.

B. Biodegradation

In an OECD 301F study, there was 62.5% degradation after 28 days (ECHA) [Kl. score = 1]. The results indicate that this substance is readily biodegradable even though it did not meet the 10-day window because the criterion does not apply to multi-component substance when assessing their ready biodegradability (ECHA) [Kl. score = 1]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental studies are available on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl). Using KOCWIN v2.00, K_{oc} values were calculated for the following constituents (ECHA) [Kl. score = 2]:

C12 fatty acid EO1: K_{oc} = 53.81

C12 fatty acid EO7: K_{oc} = 116

The K_{oc} values indicate a low adsorption potential and high potential for mobility. However, these substances also have a potential for surface active properties, which is not accounted for in the QSAR model calculations. The adsorption of non-ionic surfactants to soil is generally high as shown in experimental studies on Polysorbate 80 (CAS No. 9005-65-6) (ECHA). Consequently, sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is expected to adsorb to soil or sediments similar to other sorbitan esters.

D. Bioaccumulation

No experimental studies are available on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl). The bioconcentration factor (BCF) was estimated using the QSAR model BCFBAF v3.01 (ECHA). Using the Arnot-Gobas method, BCF values of 1.2 to 7.1 were calculated for the main constituents. When biotransformation was excluded, the BCF values of 2.7 to 758 L/kg were obtained. These results indicated that there is extensive metabolism of Polysorbate 20, and thus the bioaccumulation potential of Polysorbate 20 is low (ECHA) [Kl. score = 2].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Polysorbate 20 is of low-to-moderate toxicity concern to aquatic life. Data to support this conclusion are discussed below.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sorbitan monolaurate, ethoxylated (1 – 6.5 moles ethoxylated).

Table 3 Acute Aquatic Toxicity Studies on Sorbitan Monolaurate, Ethoxylated (1-6.5 Moles Ethoxylated) [CAS No. 9005-64-5]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachydanio rerio	96-hr LL_{50}	>100 [WAF]	2	ECHA
Pseudokirchneriella subcapitata	72-hr EL_{50}	58.84 [WAF]	2	ECHA

Chronic Studies

The 21-day NOELR (no-observed-effect-loading-rate) for sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5] in a *Daphnia* reproduction test was 10 mg/L WAF (ECHA) [Kl. score = 2].

The 72-hr EL_{10} for sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5] to *Pseudokirchneriella subcapitata* is 19.05 mg/L WAF (ECHA) [Kl. score = 2].

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on calculate BCF values of 1.2 to 7.1, sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is >0.1 mg/L WAF. The acute EL_{50} values for sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) in fish and algae are >1 mg/L WAF. Thus, sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) does not meet the criteria for toxicity.

The overall conclusion is that sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl).

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl)	9005-64-5	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 – PBT Assessment based on PBT Framework.

2 – Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	Bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EL	Effective level
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram

LL	Lethal level
mg/L	milligrams per litre
NOELR	no-observed-effect-loading-rate
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

SORBITAN MONOOLEATE POLYOXYETHYLENE DERIVATIVE

This dossier on sorbitan monooleate polyoxyethylene derivative presents the most critical studies pertinent to the risk assessment of sorbitan monooleate polyoxyethylene derivative in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA), and the European Food and Safety Authority (EFSA, 2015). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sorbitan monooleate polyoxyethylene is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sorbitan monooleate polyoxyethylene derivative is a hydrophilic, non-ionic surfactant used as an emulsifier. It is considered a UVCB substance (substance of unknown or variable composition, complex reaction products or biological materials). Based on the substance group types evaluated, the substance is likely to biodegrade, has a low potential to bioaccumulate and, based on its non-ionic surfactant properties will adsorb to soils. Based on read across from a similar substance (sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5]), acute and chronic toxicities are relatively low.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sorbitan monooleate polyoxyethylene derivative

CAS RN: 9005-65-6

Molecular formula: Not available (UVCB substances)

Molecular weight: Not available (UVCB substances)

Synonyms: See below.

The composition of sorbitan monooleate polyoxyethylene derivative (CAS No. 9005-65-6) is unknown. The CAS No. 9005-65-6 is a generic CAS No. that can include at least the following UVCB substance groups:

1. An ethoxylated sorbitan ester of oleic acid with an average of 3 moles of ethylene oxide (e.g., PEG-3-sorbitan oleate). PubChem CID: 78382488

2. A mixture of oleate esters of sorbitol and sorbitol anhydrides, consisting predominantly of the monoester, condensed with approximately 5 moles of ethylene oxide (e.g., Polysorbate 81).

3. An ethoxylated sorbitan ester of oleic acid with an average of 6 moles of ethylene oxide (e.g., PEG-6 sorbitan oleate).

4. An ethoxylated sorbitan ester of oleic acid with an average of 20 moles of ethylene oxide (e.g., PEG-20 sorbitan oleate).

5. A mixture of oleate esters of sorbitol and sorbitol anhydrides, consisting predominantly of the monoester, condensed with approximately 20 moles of ethylene oxide (e.g., Polysorbate 80).

This dossier will include information from the following substances:

Sorbitan monooleate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-65-6]

Polysorbate 80 (CAS No. 9005-65-6)

Sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5]

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sorbitan Monooleate, Ethoxylated (1 – 6.5 Moles Ethoxylated) [CAS No. 9005-65-6]*

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	2	ECHA
Melting point	-32.7°C @ 101.3 kPa -33.9°C @ 101.3 kPa	2 2	ECHA
Boiling point	No data	-	ECHA
Density	1030 kg/m^3 @ 25°C	2	ECHA
Vapour pressure	0 Pa @ 20°C (QSAR)	2	ECHA
Partition coefficient (log K_{ow})	4.51 to 5.06 (QSAR)**	2	ECHA
Water solubility	0.035 to 0.100 g/L @ 20°C***	1	ECHA
Dissociation constant (pKa)	13.89 @ @ 20°C	2	ECHA
Viscosity	672.3 840.4 mPa s @ 20°C	2	ECHA

*Data located in REACH database for dehydrated sorbitol, C18 (unsaturated) fatty acid esters, ethoxylated (EC No. 701-203-3).

**QSAR (KOWWIN v1.68): sorbitan monooleate, ethoxylated 5EO and sorbitan monooleate, ethoxylated 3EO, respectively.

***Sorbitan monooleate, ethoxylated 3EO: ~100 mg/L; sorbitan monooleate, ethoxylated 5EO: ~35 mg/L.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sorbitan monooleate polyoxyethylene derivative.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

The substance is likely to biodegrade, has a low potential to bioaccumulate and, based on it non-ionic surfactant properties will adsorb to soils. The data supporting these conclusions are discussed below.

B. Biodegradation

In an ISO Standard 14593 ready biodegradation test, degradation of Tween 81 (CAS No. 9005-65-6) was 61% after 28 days, indicating ready biodegradability (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for sorbitan monooleate polyoxyethylene derivative. Using KOCWIN v2.00, the estimated K_{oc} values for the main components in sorbitan monooleate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-65-6] based on the molecular connectivity index (MCI) ranged from 794 to 1,259 L/kg (ECHA). Based on these estimated K_{oc} values, the substance is likely to adsorb to soil or sediments.

Further, the molecular structure indicates a potential of surface-active properties, which are not taken into account by the QSAR model calculations. As a result, the adsorption of non-ionic surfactants to soil is generally high (ECHA). Based on these considerations, there is a low potential for mobility.

D. Bioaccumulation

There are no experimental bioaccumulation studies on sorbitan monooleate polyoxyethylene derivative. The bioaccumulation potential was estimated for sorbitan monooleate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-65-6] using BCFBAF v3.01 (Arnot-Gobas method, including biotransformation). The calculated BCF values were 12.6 to 14.6 L/kg. When biotransformation was excluded, the BCF values were 18.6 to 42.8 L/kg (ECHA). Thus, sorbitan monooleate polyoxyethylene derivative has a low potential for bioaccumulation.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Based on read across from a similar substance, acute and chronic toxicities are relatively low. Data to support this conclusion are discussed below.

B. Aquatic Toxicity

Acute Studies

There are no adequate aquatic toxicity studies on sorbitan monooleate polyoxyethylene derivative. Aquatic toxicity data has been read-across from sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5]; see Table 3.

Table 3 Acute Aquatic Toxicity Studies on Sorbitan Monolaurate, Ethoxylated (1-6.5 Moles Ethoxylated) [CAS No. 9005-64-5]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachydanio rerio	96-hr LL_{50}	>100 [WAF]	2	ECHA
Pseudokirchneriella subcapitata	72-hr EL_{50}	58.84 [WAF]	2	ECHA

Chronic Studies

The 21-day NOELR (no-observed-effect-loading-rate) for sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5] in a *Daphnia* reproduction test was 10 mg/L WAF (ECHA) [Kl. score = 2].

The 72-hr EL_{10} for sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5] to *Pseudokirchneriella subcapitata* is 19.05 mg/L WAF (ECHA) [Kl. score = 2].

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sorbitan monooleate polyoxyethylene derivative is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on the estimated BCF values of 12.6 to 14.6 L/kg, sorbitan monooleate polyoxyethylene derivative does not meet the criteria for bioaccumulation.

The chronic toxicity data on sorbitan monooleate polyoxyethylene derivative are >0.1 mg/L WAF. The acute EL_{50} values for sorbitan monooleate polyoxyethylene derivative are >1 mg/L WAF. Thus, sorbitan monooleate polyoxyethylene derivative does not meet the criteria for toxicity.

The overall conclusion is that sorbitan monooleate polyoxyethylene derivative is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sorbitan monooleate polyoxyethylene derivative.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sorbitan monooleate polyoxyethylene derivative	9005-65-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	USEPA bioconcentration factor/bioaccumulation factor estimation model
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EFSA	European Food and Safety Authority
EL	Effective level
EU	European Union

g/L	grams per litre
ISO	International Organization for Standards
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LL	Lethal level
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal - second
NOELR	no-observed-effect-loading-rate
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	Water accommodated fraction

ACETIC ACID

This dossier on acetic acid presents the most critical studies pertinent to the risk assessment of acetic acid in its use in hydraulic fracturing fluids and water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Acetic acid is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Acetic acid is a flammable liquid. It readily dissociates in aqueous media to the acetate (H_3C2O_2-) and hydrogen (H+) ions. The acetate ion is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil. Acetic acid is of moderate toxicity to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion. The acetate ion is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Acetic acid

CAS RN: 64-19-7

Molecular formula: $C_2H_4O_2$

Molecular weight: 60.1 g/mol

Synonyms: Acetic acid, ethanoic acid, ethylic acid, methane carboxylic acid, vinegar acid

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Acetic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid with a pungent odour.	2	ECHA
Melting Point	16.64°C @ 101.3 kPa	2	ECHA
Boiling Point	117.9°C @ 101.3 kPa	2	ECHA
Density	1040 kg/m^3 @ 25°C	2	ECHA
Vapour Pressure	2079 Pa @ 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-0.17 @ 20°C	2	ECHA
Water Solubility	602.9 g/L @ 25°C	2	ECHA
Viscosity	1.056 mPa s @ 25°C	2	ECHA
Dissociation constant (pKa)	4.756 @ 25°C	2	ECHA

Acetic acid readily dissociates in aqueous media to the acetate ($H_3C2O_2^-$) and hydrogen (H^+) ions.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for acetic acid.

Based on an assessment of environmental hazards, NICNAS identified acetic acid as a chemical of low concern to the environment (DoEE, 2017a). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

The acetate ion of acetic acid is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Partitioning

The pKa of acetic acid is 4.76, indicating that this substance will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts (PubChem).

Volatilization of acetic acid from water and moist soil surfaces is not expected to be an important fate process given a Henry's Law constant of 0.21 Pa-m^3/mole (ECHA). Acetic acid is expected to volatilize from dry soil surfaces based upon its vapour pressure.

Hydrolysis is not expected to be an important environmental fate process since this substance lacks functional groups that hydrolyze under environmental conditions(PubChem).

C. Biodegradation

Acetic acid was readily biodegradable in a non-acclimated freshwater study. Degradation was 96% after 20 days (Price et al., 1974; ECHA) [Kl. score = 2]. Acetic acid is also readily biodegradable under anaerobic conditions (Kameya et al., 1995) [Kl. score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017b).

D. Environmental Distribution

No experimental data are available for acetic acid. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values from log K_{ow} and the molecular connectivity index (MCI) are 1.153 and 1.0 L/kg, respectively. Based on these values, acetic acid has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

Acetic acid is highly soluble in water and dissociates completely in aqueous solution to acetate and its hydrogen ion. However, the chemistry of the receiving water compartment, such as its pH and the presence of metal ions, may affect the speciation and partitioning of this substance and its buffering capacity (DoEE, 2017c).

E. Bioaccumulation

There are no bioaccumulation studies on acetic acid. Bioaccumulation of acetic acid is not expected to occur because acetic acid dissociates completely in aqueous solution to acetate and its hydrogen ion. Both ions are ubiquitous in the environment. Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Acetic acid is of moderate acute toxicity concern to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion. The acetate ion is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 presents the results of acute aquatic toxicity studies on acetic acid and potassium acetate.

Table 3 Acute Aquatic Toxicity Studies on Acetic Acid and Potassium Acetate

Test Substance	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Potassium acetate	*Oncorhynchus mykiss*	96-hour LC_{50}	>300.82*	2	ECHA
Potassium acetate	*Danio rerio*	96-hour LC_{50}	>300.82*	2	ECHA
Acetic acid	*Oncorhynchus mykiss*	96-hour LC_{50}	64.8 (measured)	4	ECHA
Acetic acid	*Oncorhynchus mykiss*	96-hour LC_{50}	31.3 – 67.6	4	ECHA
Potassium acetate	*Daphnia magna*	48-hour EC_{50}	>300.82*	2	ECHA
Acetic acid	*Daphnia magna*	48-hour EC_{50}	79.5 (measured)	4	ECHA
Acetic acid	*Daphnia magna*	48-hour EC_{50}	18.9 (measured)	4	ECHA
Acetic acid	*Desmodesmus subspicatus*	72-hour EC_{50}	486.5	4	ECHA

*As the acetate ion.

Chronic Studies

In a 21-day fish (*Oncorhynchus mykiss*) chronic study, the measured NOEC values for 60% and 100% acetic acid were 57.2 and 34.3 mg/L, respectively (ECHA). [Kl. score = 4]

In a 21-day *Daphnia* reproduction study, the measured NOEC for 60% and 100% acetic acid were 80 and 31.4 mg/L, respectively (ECHA). [Kl. score = 4]

In a 21-day *Daphnia* reproduction study, the measured NOEC for 100% acetic acid was 22.7 mg/L (ECHA). [Kl. score = 4]

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARCTERSTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Acetic acid is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Bioaccumulation of acetic acid is not expected to occur because acetic acid dissociates completely in aqueous media to acetate and its hydrogen ion. Both ions are ubiquitous in the environment.

Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways. The log K_{ow} for acetic acid is -0.17. Thus, acetic acid does not meet the screening criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on acetic acid are >0.1 mg/L. The EC_{50} values for potassium acetate are > 1 mg/L. Thus, acetic acid does not meet the criteria for toxicity.

The overall conclusion is that acetic acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for acetic acid.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Acetic Acid	64-19-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
gm/mol	
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Acetylene

This dossier presents the most critical studies pertinent to the risk assessment of acetylene as it relates to its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all the available data. Most of the information presented in this dossier was obtained from the ECHA database which provides information on chemicals that have been registered under the EU REACH (ECHA) framework. Where possible, the study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion- Acetylene is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

During a carbide lag test, acetylene gas is produced when calcium carbide reacts with water in the drilling fluid. Acetylene is commonly used as a tracer gas for this purpose. It circulates with the drilling fluid until it reaches the surface, where it is detected and captured at the gas trap.

Acetylene is a flammable, colourless, gas that is soluble in water. As acetylene is a gas at standard temperature and pressure, biodegradation is not considered relevant. It is not expected to bioaccumulate and has a low potential to adsorb to soil or suspended sediments. Volatilisation is expected to be an important fate process.

Acetylene is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL AND IDENTIFICATION

Chemical Name (IUPAC): Acetylene

CAS RN: 74-86-2

Molecular formula: C_2H_2

Molecular weight: 26.038 g/mol

Synonyms: Ethyne

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Acetylene

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless gas	2	ECHA
Melting Point	-80.7 °C @ 101.3 kPa	2	ECHA
Boiling Point	-85 °C @ 101.3 kPa	2	ECHA

Property	Value	Klimisch score	Reference
Density	380 kg/m^3 @ 25 °C	2	ECHA
Vapour Pressure	4.54 x10^6 Pa @ 22 °C	2	ECHA
Partition Coefficient (log K_{ow})	0.37 @ 25 °C	2	ECHA
Water Solubility	1.2 g/L @ 20 °C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances-ACIS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for acetylene.

Table 2 Existing International Controls

Convention, Protocol, or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE PROPERTIES

A. Summary

Acetylene is a flammable, colourless, gas that is soluble in water. As acetylene is a gas at standard temperature and pressure, biodegradation is not considered relevant. It is not expected to bioaccumulate and has a low potential to adsorb to soil or suspended sediments. Volatilisation is expected to be an important fate process.

B. Partitioning

Acetylene is a flammable, colourless, gas that is soluble in water. Based upon a Henry's Law constant of 2,200 Pa m^3/mol (ECHA), it is expected to volatilise from water and moist soil surfaces. It is also expected to volatilise from dry soil surfaces based upon its vapour pressure.

Volatilisation for surface waters will predictably be rapid: calculations based on Henry's Law constant indicates that the volatilisation half-life will be less than 6 days in a water body up to10 metres deep and

similar calculations using the EPISuite v.4.0 model predicts half-lives of 32 minutes and 49 hours in rivers and lakes, respectively (1m depth, wind velocity 5 m/sec and 0.5 m/sec, respectively). If released into surface water, volatilisation will therefore ensure rapid removal of acetylene into the atmospheric compartment. Once in the atmosphere, acetylene is expected to be rapidly removed by photooxidation (ECHA).

C. Biodegradation

As acetylene is a gas at standard temperature and pressure, biodegradation is not considered relevant or applicable (ECHA).

D. Environmental Distribution

No experimental data are available for acetylene. Using KOCWIN in EPISuite™ (USEPA, 2019), the estimated K_{oc} value from log K_{ow} of 0.37 is2.093 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 13.22 L/kg. Thus, acetylene has a high potential for mobility in soil. If released into water, acetylene is also not expected to adsorb to suspended solids and sediment in water; and, as noted earlier, volatilisation is expected to be an important fate process (ECHA).

E. Bioaccumulation

A bioconcentration factor of 3 was calculated for acetylene based on its log K_{ow} of 0.37 (ECHA)[KI.Score=2]. This calculated BCF factor suggests that acetylene will not bioaccumulate in the aquatic environment.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Acetylene is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Measured data are not available for the aquatic toxicity endpoints. Due to the practical difficulties associated with the ecotoxicity testing of gases (i.e., maintaining exposure concentrations) the use of QSAR toxicity estimates is an appropriate alternative. The ECOSAR v1.00 model is a reliable and appropriate QSAR model to apply to acetylene (ECHA).

Acute Studies

Table 3 lists the results of the QSAR acute toxicity estimates for acetylene.

Table 3 Acute Aquatic Toxicity Studies on Acetylene

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Freshwater Fish	96-hr LC_{50}	545	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnids	48-hr LC_{50}	242	2	ECHA
Freshwater Algae	96-hr EC_{50}	57	2	ECHA

Chronic Studies

There are no reliable chronic toxicity studies available for acetylene.

C. Terrestrial Toxicity

Measured data are not available for the terrestrial toxicity endpoints. Similar to the discussion presented for aquatic toxicity testing, the ECOSAR v1.00 model is a reliable and appropriate QSAR model to apply to acetylene (ECHA).

Table 4 lists the results of the QSAR terrestrial toxicity estimates for acetylene.

Table 4 Terrestrial Toxicity Studies on Acetylene

Test Species	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Earthworm	14-d LC_{50}	67	2	ECHA

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

The biodegradation endpoint is not relevant for acetylene. As such acetylene does not meet the screening criteria for persistence.

Based on a log K_{ow} of 0.37, acetylene is not expected to bioaccumulate. Thus, it does not meet the screening criteria for bioaccumulation.

No chronic aquatic toxicity data exist on acetylene; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates, and algae. Therefore, acetylene does not meet the screening criteria for toxicity.

The overall conclusion is that acetylene is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for acetylene.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Acetylene	74-86-2	Not a PBT	No	No	NA	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS, AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IMAP	Inventory Multitiered Assessment and Prioritisation
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration

mg/kg	milligrams per kilogram
NOEC	no observed effective concentration
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

ALCOHOLS, C12-15, ETHOXYLATED

This dossier on alcohols, C12-15, ethoxylated presents the most critical studies pertinent to the risk assessment of alcohols, C12-15, ethoxylated in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products: Alcohol Ethoxylates (HERA, 2009), and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Alcohols, C12-15, ethoxylated is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x-y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerisation is indicated by the subscript (n) which indicates the average number of ethylene oxide units. Alcohols, C12-15, ethoxylated (CAS No. 68131-39-5) has an average number of 1 to 2.5 moles of ethylene oxide units.

Alcohols, C12-15, ethoxylated are readily biodegradable, are not likely to sorb to sediments or soil, have low potential to bioaccumulate or bioconcentrate and are of low toxicity to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Alcohols, C12-15, ethoxylated

CAS RN: 68131-39-5

Molecular formula: $(C_2H_4O)1\text{-}3(CH_2)10\text{-}13C_2H_6O$

Molecular weight: Not available

Synonyms: Alcohols, C12-15, ethoxylated

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Alcohols, C12-15, Ethoxylated (1 to 2.5 moles ethoxylated)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear liquid with a rancid odour*	2	ECHA
Melting Point	7.22°C (pressure not provided)	2	ECHA
Boiling Point	ca. 287°C @ 101.3 kPa	1	ECHA
Density	926 kg/m^3 @ 15.56°C	1	ECHA
Vapour Pressure	Negligible	-	ECHA
Partition coefficient (log K_{ow})	5.06* @ 25°C	2	ECHA
Water Solubility	0.007 – 0.063 g/L @ 25°C	2	ECHA
Dissociation constant (pKa)	No dissociation	-	ECHA
Viscosity	28.1 mPa s (dynamic) @ 20°C	2	ECHA

*Based on alcohols, C12-14, ethoxylated (1 to 2.5 EO) [CAS No. 68439-50-9]

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for alcohols, C12-15, ethoxylated.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Alcohols, C12-15, ethoxylated is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for adsorption to soil and sediment.

B. Biodegradation

Alcohols, C12-15, ethoxylated is readily biodegradable. In an OECD 301B test, degradation was 72% in 28 days, but failed the 10-day window (ECHA) [Kl. score = 1].

An alcohol, C12-15, ethoxylated (7 EO) degraded 80 to 88% in 28 days when tested using a shake-flask CO_2-evolution test method (ECHA) [Kl. score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for alcohols, C12-15, ethoxylated. Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K_{oc} values for surrogates of alcohols, C12-15, ethoxylated are:

C12 linear alcohol, ethoxylated (2 EO): 279.5 L/kg (MCI) and 464.2 L/kg (K_{ow})

C15 linear alcohol, ethoxylated (2 EO): 1,691 L/kg (MCI) and 3,018 L/kg (K_{ow})

Based on these values, the substance has a moderate potential for adsorption to soil or sediments and a low potential for mobility.

D. Bioaccumulation

The potential for bioaccumulation of alcohol ethoxylates is considered low due to the biotransformation and excretion of the substance. The BCF values for alcohol ethoxylates in fathead minnows have been reported to range from <5 to 387.5 (Toll et al., 2000). The uptake rates varied from 330 to 1660 (L x kg/day) and elimination rates varied from 3.3 to 59 per day (Toll et al., 2000). The high concentrations in fish is thought to be prevented by an efficient biotransformation of the alcohol ethoxylates, leading to a high elimination rate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Alcohol, C12-15, ethoxylated has moderate chronic toxicity concern to aquatic life.

B. Aquatic Toxicity

In developing a water quality guideline for alcohol ethoxylates (ANZG, 2018), the toxicity data was normalised for a specific alkyl chain length or a specific number of ethoxylate (EO) groups. The NOECs listed below were normalised to an alkyl chain length of C13.3 and EO of 8.2.

Freshwater fish: 2 species, 720 to 1,500 mg/L.

Freshwater crustaceans: 2 species, 590 to 860 mg/L.

Freshwater rotifers: 1 species, *Brachionus calyciflorus*, 1,300 mg/L

Freshwater algae, diatoms and blue-green algae: 6 species, 200 to 8,700 mg/L.

Freshwater mesocosms: 4 NOEC data for multiple species tests were 80, 80, 320 and 330 mg/L, although replication was insufficient to meet OECD (1992) requirements. Normalised data were 380, 380, 320 and 1,520 mg/L.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Alcohols, C12-15, ethoxylated is readily biodegradable and thus does not meet the screening criteria for persistence.

The bioconcentration factors (BCF) in fish for ethoxylated alcohols (which includes alcohols, C12-15, ethoxylated) have been reported to range from <5 to 387.5. Thus, alcohols, C12-15, ethoxylated does not meet the screening criteria for bioaccumulation.

The chronic NOEC values for alcohols ethoxylates are >0.1 mg/L. Thus, alcohols, C12-15, ethoxylated do not meet the criteria for toxicity.

Thus, alcohols, C12-15, ethoxylated is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for alcohols, C12-15, ethoxylated.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Alcohols, C12-15, ethoxylated	68131-39-5	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

ANZG. 2018. Australian and New Zealand Guidelines for Fresh and Marine Water Quality. Australian and New Zealand Governments and Australian state and territory governments, Canberra ACT, Australia. Available at www.waterquality.gov.au/anz-guidelines

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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Toll, J., Haller, M., Labee, E., Verweij, M., and Sijm, D.T.H.M. (2000). Toxicology and Chemistry, 19 646–653.

USEPA. (2018). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of9Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

B. Abbreviations and Acronyms

°C	degrees Celsius
AE	alcohol ethoxylates
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Government
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EO	ethoxylate
EU	European Union
g/l	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/mg^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
MCI	molecular connectivity index
mg/L	milligrams per litre
mPA s	millipascal second
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

ALIPHATIC ALCOHOL ETHOXYLATE

This dossier on aliphatic alcohol ethoxylate presents the most critical studies pertinent to the risk assessment of these substances in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Aliphatic alcohol ethoxylate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Aliphatic alcohol ethoxylate is an organic UVCB compound. It is readily biodegradable, does not bioaccumulate and is of low aquatic and terrestrial toxicity concern.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Poly(oxy-1,2-ethanediyl), α-butyl-ω-hydroxy-

CAS RN: 9004-77-7

Molecular formula: $(C_2H_4O)nC_4H_{10}O$

Molecular weight: 118.17 g/mol (Substance is a UVCB)

Synonyms: 2-butoxyethanol, butylcellosolve, ethyleneglycol monobutyl ether, n-butoxyethanol, n-butoxyethanol sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of aliphatic alcohol ethoxylate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	liquid	2	ECHA
Melting Point	-30 °C @101.3 kPa	2	ECHA
Boiling Point	278 °C @ 101.3 kPa	2	ECHA
Density	989 kg/m^3 @ 20 °C	2	ECHA
Vapour Pressure	<1Pa @ 20°C	2	ECHA-
Partition Coefficient (log K_{ow})	0.44 @ 20°C	2	ECHA
Water Solubility	989 g/L @ 20°C	2	ECHA
Dissociation Constant (pKa)	14.9 @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Viscosity	9.4 mPa s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for aliphatic alcohol ethoxylate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Aliphatic alcohol ethoxylate is readily biodegradable and has a low tendency to bind to soil or sediment. It is not expected to bioaccumulate.

B. Partitioning

Aliphatic alcohol ethoxylate is highly soluble in water. Based on the Henry's Law Constant for the monomer of 1.60 X 10^{-6} atm-m^3/mol, it is expected to volatilise from water and moist soil surfaces. It is expected to volatilise slowly from dry soil surfaces based upon its vapour pressure. After evaporation or exposure to air, modelling of 2 -(2 -butoxyethoxy)ethanol (CAS No. 112-34-5), a representative molecule for this UVCB substance, predicts that it is likely to undergo indirect photolysis through hydroxyl radical reaction at a fast rate, with an estimated half life of 2.5 hours (0.21 days) at an OH concentration of 1.5million OH/cm^3 and a 12 hour day) (ECHA).

Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyse under environmental conditions (PubChem).

C. Biodegradation

In a guideline (OECD 301D) and GLP ready biodegradability study, a substance corresponding to the description "Ethanol, 2-butoxy- manufacture of, by-products from" gave a positive result (>60%

degradation relative to the COD value) with a maximum of 76% biodegradation recorded on day 28. In a similar GLP study to the same protocol, the substance "Poly(oxy-1,2-ethanediyl), α-butyl-ω-hydroxy" attained 69% degradation after 28 days [KI Score = 2](ECHA). Thus, aliphatic alcohol ethoxylate is considered to be readily degradable.

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No studies were available for the substance. Based on a log K_{ow} of 0.44, the substance is expected to have a low potential for adsorption and have very high mobility in soil. If released to water, based on its high water solubility value, it is likely to remain in water and not adsorb to suspended solids or sediment.

E. Bioaccumulation

No studies were available as the substance. Aliphatic alcohol ethoxylate has a low K_{ow} (0.44); and, therefore, bioaccumulation is expected to be low.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Aliphatic alcohol ethoxylate is of low toxicity concern to aquatic and terrestrial organisms. Details are provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on aliphatic alcohol ethoxylate.

Table 3 Acute Aquatic Toxicity Studies on Aliphatic alcohol ethoxylate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Turbot (marine species)	96-hour LC_{50}	1,800 mg/L	2	ECHA
Daphnia magna	48-hour EC_{50}	>3200mg/l	2	ECHA
Selenastrum capricornutum	72 hour EC_{50}	2,490mg/l	2	ECHA

Chronic Studies

No chronic studies were identified.

C. Terrestrial Toxicity

No studies were identified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Significant biodegradation of aliphatic alcohol ethoxylate is expected. For the purposes of this PBT assessment, the persistence criteria are not met.

Based on a measured log K_{ow} of 0.44, aliphatic alcohol ethoxylate does not meet the screening criteria for bioaccumulation.

No chronic studies were identified. Acute aquatic toxicity data are >1 mg/L. Thus, aliphatic alcohol ethoxylate does not meet the screening criteria for toxicity.

The overall conclusion is that aliphatic alcohol ethoxylate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for aliphatic alcohol ethoxylate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Aliphatic alcohol ethoxylate	9004-77-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
PEC	Predicted exposure concentrations

REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

ALUMINIUM OXIDE

This dossier on aluminium oxide presents the most critical studies pertinent to the risk assessment of aluminium oxide in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Aluminium oxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Aluminium oxide or alumina, (Al_2O_3), is an inert, odourless, white amorphous material often used in industrial ceramics. Due to its outstanding properties, alumina has contributed to a significant number of life-extending and society-enhancing applications. It is of little toxicological concern to humans and the environment.

Due to aluminium oxide's hardness, bio-inertness and chemical properties, it is a preferred material for bearings in hip replacements, as prostheses, bionic implants, prosthetic eye substitutes, tissue reinforcements, dental crowns, abutments, bridges and other dental implants. It is also used in lab equipment and tools like crucibles, furnaces and other labware.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): oxo[(oxoalumanyl)oxy]alumane

CAS RN: 1344-28-1

Molecular formula: Al_2O_3

Molecular weight: 101.961 g/mol

Synonyms: Bauxite, Ceramic-Alumina, Corundum, Oxide, Aluminium

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Aluminium Oxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, odourless powder	1	ECHA
Melting Point	2,054°C (pressure not provided)	1	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	2,977°C @101.3 kPa (assumed pressure)	1	ECHA
Density	>3970 - < 3990 kg/m³@ 20°C	1	ECHA
Vapour Pressure	0 Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	The study does not need to be conducted because the substance is inorganic.	-	ECHA-
Water Solubility	0 g/L@ 20°C	1	ECHA
Dissociation Constant (pKa)	The study does not need to be conducted because the substance is insoluble	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for aluminium oxide.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Aluminium oxide is an inorganic substance that is not subject to biodegradation, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Biodegradation

Aluminium oxide is an inorganic substance. According to Annex VII of the REACH regulations (ECHA), biodegradation testing for inorganic chemicals is not required.

C. Environmental Distribution

Environmental distribution or mobility of a substance is mainly driven by the adsorption potential. The potential of aluminium for adsorption to sediment and soil particles is mainly driven by its speciation and the concentration of dissolved organic carbon (DOC) (ECHA).

For evaluation of adsorption at different pH-levels a chemical simulation was performed. In the stimulation, the amount of aluminium bound to particles as a result of surface complexation (i.e. adsorption) was pH dependent, but was typically less than 8% of the total aluminium at pH 6, and was further reduced to below 1% at pH values above 7. This distribution was similar in both soft and hard waters. The corresponding Log Kd values for this distribution are between 3 and 5. Very similar results were obtained with higher DOC concentrations of 4 mg/L (ECHA)[Kl Score =2].

D. Bioaccumulation

The available evidence shows the absence of aluminium biomagnification across trophic levels both in aquatic and terrestrial food chains. The existing information suggests not only that aluminium does not biomagnify, but rather that it tends to exhibit biodilution at higher trophic levels in the food chain (ECHA) [Kl Score =2].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Aluminium oxide is of low acute toxicity concern to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion.

B. Aquatic Toxicity

Acute Studies

Data available on aluminium oxide have been generated to demonstrate bioavailability of aluminium in acid water. Adequate studies were found to evaluate the intrinsic toxicity of aluminium oxide. Nonetheless, aluminium oxide is not expected to pose a substantial acute toxicity concern to aquatic receptors (ECHA) [Kl Score =2].

Chronic Studies

No studies are available.

Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Aluminium oxide is an inorganic mineral. Thus, biodegradation is not applicable to this substance. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to aluminium oxide.

Aluminium oxide is a naturally inorganic substance and as an inorganic complex is not expected to bioaccumulate. Thus, aluminium oxide does not meet the screening criteria for bioaccumulation.

Thus, aluminium oxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for aluminium oxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Aluminium oxide	1344-28-1	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
mg/L	milligrams per litre
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Amylodextrin

This dossier presents the most critical studies pertinent to the risk assessment of amylodextrin as it relates to its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all the available data. As there are no available studies for amylodextrin, this dossier is based on information obtained from similar read-across substance starch (CAS No. 9005-25-8). Where possible, the study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion- Amylodextrin is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Amylodextrin is a short chain amylose that is produced by enzymatic hydrolysis of alpha-1,6 glycosidic bonds or debranching of amylopectin. Amylodextrin is a form of dextrin which is a low molecular weight carbohydrate polymer that is structurally characterized by glucose (D) units linked by glycosidic bonds. Dextrins are created when starch is heated in the presence of small amounts of moisture and an acid. Dextrins occur naturally in the human digestive system via the enzyme amylases which are catalysed by hydrolysis of starch in the human mouth.

Amylodextrin is expected to be biodegradable and does not bioaccumulate. Amylodextrin is not toxic to aquatic organisms.

2 CHEMICAL AND IDENTIFICATION

Chemical Name (IUPAC): (2*R*,3*S*,4*S*,5*R*,6*R*)-2-(hydroxymethyl)-6-[(2*R*,3*S*,4*R*,5*R*,6*S*)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol

CAS RN: 9005-84-9

Molecular formula: $C_{12}H_{22}O_{11}$

Molecular weight: 342.30 g/mol

Synonyms: Amylodextrin; starch, soluble; alpha-maltose; maltose

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Amylodextrin

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid	-	PubChem
Melting Point	240 °C (pressure not provided)	-	PubChem
Boiling Point	591.67 °C (pressure not provided)	-	EPISUITE

Property	Value	Klimisch score	Reference
Density	Not Available	-	-
Vapour Pressure	$7.1x10^{-15}$ Pa @ 25 °C	-	EPISUITE
Partition Coefficient (log K_{ow})	-5.12	-	EPISUITE
Water Solubility	52.2 g/L @ 20 °C	-	EPISUITE

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances-ACIS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for amylodextrin.

NICNAS has assessed amylodextrin in an IMAP Tier 1 assessment and it was concluded that this chemical poses no unreasonable risk to human health or the environment. It was also identified as a polymer of low concern[1].

Table 2 Existing International Controls

Convention, Protocol, or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE PROPERTIES

Amylodextrin is a form of dextrin, which is a low molecular weight carbohydrate polymer that is structurally characterized by glucose (D) units linked by glycosidic bonds. Dextrins are created when starch is heated in the presence of small amounts of moisture and an acid.

Amylodextrin is soluble in water. As a carbohydrate polymer, the substance is expected to be biodegradable.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9005-84-9%2C+

No bioaccumulation studies have been conducted on amylodextrin. A bioconcentration factor of 3.162 L/kg was estimated for the chemical using the log K_{ow} (-5.12) and the regression-based method in EPISUITE (USEPA, 2019). Based on this BCF, amylodextrin is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Amylodextrin is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Aquatic toxicity data is not available for amylodextrin or dextrin (CAS No. 9004-53-9). Therefore, available aquatic toxicity data is provided for similar substance starch (CAS No. 9005-25-8).

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on starch.

Table 3 Acute Aquatic Toxicity Studies on Starch (CAS No. 9005-25-8)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Orthopristis chrysoptera (pigfish)	96-h LC_{50}	>5,000	4	US EPA
Bairdiella chrysoura (silver perch)	96-h LC_{50}	>5,000	4	US EPA
Lagodon rhomboids (pinfish)	96-h LC_{50}	>5,000	4	US EPA

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Amylodextrin as a carbohydrate polymer is expected to be readily biodegradable. Therefore, it does not meet the screening criteria for persistence.

Based on an estimated log K_{ow} of -5.12, amylodextrin does not meet the screening criteria for bioaccumulation.

There are no chronic toxicity studies on amylodextrin. The acute LC_{50} values for read-across similar substance starch are >1 mg/L. Therefore, amylodextrin does not meet the screening criteria for toxicity.

Therefore, amylodextrin is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for amylodextrin.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Amylodextrin	9005-84-9	Not a PBT	No	Yes	No	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS, AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

Eduok, M.U., Umoren, A.S., (2016). Application of carbohydrate polymers as corrosion inhibitors for metal substrates in different media: A review. Amylodextrin - an overview | ScienceDirect Topics

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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USEPA. ECOTOX Database. Available at: http://cfpub.epa.gov/ecotox/.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre

IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

BARIUM SULFATE

This dossier on barium sulfate presents the most critical studies pertinent to the risk assessment of barium sulfate in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Barium sulfate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Barium sulfate is an inorganic compound. It is partially soluble in water, dissociating into barium (Ba^{2+}) and sulfate (SO_3^{2-}) ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. Barium sulfate is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): barium (2+) sulfate

CAS RN: 7727-43-7

Molecular formula: $BaSO_4$

Molecular weight: 233.39 g/mol

Synonyms: Barite, Baritop, Barium Sulfate (2:1),E Z CAT, Micropaque Oral, Sulfate, Barium

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Barium Sulfate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White powder	1	ECHA
Melting Point	approx. 1600 °C (pressure not provided)	2	ECHA
Boiling Point	-	-	-
Density	4500 kg/m^3 @ 20 °C	2	ECHA
Vapour Pressure	-	-	-
Partition Coefficient (log K_{ow})	-	-	-
Water Solubility	0.0031 g/L at 25°C at pH 9	1	ECHA

Property	Value	Klimisch score	Reference
Dissociation constant (pKa)	-	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for barium sulfate.

NICNAS has assessed barium sulfate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Based on an assessment of environmental hazards, NICNAS identified barium sulfate as a chemical of low concern to the environment (DoEE, 2017a). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

As an inorganic substance, barium sulfate is expected to disassociate in the environment to its respective cation and anion as limited by its aqueous solublity and pH.

B. Biodegradation

Barium sulfate is an inorganic substance. According to Annex VII of the REACH regulations (ECHA), biodegradation testing for inorganic chemicals is not required.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7727-43-7%2C+

C. Environmental Distribution

Barium sulfate has low solubility in water. Under typical environmental conditions, barium sulfate will undergo limited dissolution and dissociation into its constituent ions. Barium cations and sulfate anions are naturally ubiquitous substances that are present in all environmental compartments and subject to environmental transport processes. As a result, these substances are expected to move to soil, sediment or water compartments upon release (DoEE, 2017b).

D. Bioaccumulation

An environmental release of barium sulfate is not expected to result in significant release of ionic barium in a bioavailable form (DoEE, 2017). If present, barium bioconcentration and bioaccumulation is considered negligible. Calculated BCF values of fish (whole body) were situated between 37.6 and 98.8 (geomean of 4 values: 65.6) (Nakamoto and Hassler, 1992). Whole-body concentrations are significantly higher than reported soft tissue concentrations due to the fact that barium can replace calcium in the bones and hard tissue parts. In addition, the data indicate a certain degree of homeostatic control of internal barium levels by fish. Limited information on transfer of barium through the food chain indicates that barium does not biomagnify in aquatic food chains (ECHA) [Kl Score = 2].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Barium sulfate is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on barium sulfate.

Table 3 Acute Aquatic Toxicity Studies on Barium Sulfate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hour LC_{50}	> 3.5 mg/L (BaCl2)	1	ECHA
Daphnia magna	48-hour EC_{50}	14.5 mg Ba/L	1	ECHA

Chronic Studies

One reliable long term toxicity study for a fish species - the zebrafish *Danio rerio* - was conducted. No effect (mortality) was noted at the highest test concentration of nominal 100 mg barium dichloride dihydrate/L (ECHA) [Kl. score = 1].

Two reliable chronic toxicity studies were identified. the first study reported a 21-day EC_{16} of 5.8 mg Ba/L (nominal values), which can be used for the estimation of a NOEC-value of 2.9 mg/L (i.e., EC16/2; ECHA, 2008). The second data point was generated for the marine invertebrate *Cancer anthonyi*. A nominal, 7-day NOEC of 10 mg Ba/L was reported for the endpoint embryonal hatching.

C. Terrestrial Toxicity

Table 4 lists the results of terrestrial toxicity studies conducted on barium sulfate.

Table 4 Terrestrial Toxicity Studies on Barium Sulfate

Test Species	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Eisenia foetida	14-day LC_{50} NOEC	258	2	ECHA
E. crypticus	14-day EC_{50} NOEC	433	2	ECHA
Folsomia candida	Long-term NOEC	211	2	ECHA

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Barium sulfate is an organic salt that dissociates to barium and sulfate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both barium and sulfate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Based on calculated BCFs between 37.6 L/kg and 98.8 L/kg for barium ions, barium sulfate does not meet the screening criteria for bioaccumulation.

Both chronic and acute aquatic toxicity data are >1 mg/L. Thus, barium sulfate does not meet the screening criteria for toxicity.

The overall conclusion is that barium sulfate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for barium sulfate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Barium sulfate	7727-43-7	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE].. (2017a). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

DoEE. (2017b). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

Nakamoto RJ and Hassler, TJ. (1992). Selenium and other trace elements in bluegills from agricultural return flows in the San Joaquin Valley, California. Arch.Environ.Contam.Toxicol. 22, 88-98; cited in ECHA.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration

ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimish scoring system
kPa	kilopascal
LC	lethal concentration
L/kg	litres per kilogram
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
µg	micrograms

BENTONITE

This dossier on bentonite presents the most critical studies pertinent to the risk assessment of this substance in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Bentonite is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Bentonite is a clay generated frequently from the alteration of volcanic ash, consisting predominantly of smectite minerals, usually montmorillonite. It is conventionally used as a mud constituent for oil and water well drilling. Its roles are mainly to seal the borehole walls, to remove drill cuttings and to lubricate the cutting head.

Bentonite is inorganic, non-toxic and non-irritating. It is not considered hazardous on skin contact as it is employed in cosmetics and skin products as a suspender.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): dialuminum;disodium;oxygen(2-);silicon(4+);hydrate

CAS RN: 1302-78-9

Molecular formula: $Al_2H_2Na_2O_{13}Si_4$ as sodium form of colloidal clay, containing mainly montmorillonite)

Molecular weight: 422.29 g/mol (as sodium bentonite)

Synonyms: Albagel Premium USP 4444, Bentonite magma, Bentonite 2073, Bentopharm, CI 77004, E558, HI-Gel, HI-Jel, Imvite I.G.B.A., Magbond, mineral sopa, Montmorillonite, Panther creek bentonite, soap clay, Southern bentonite, taylorite, Tixoton, Veegum HS, Volclay, Volclay Bentonite BC, and Wilkinite

3 PHYSICO-CHEMICAL PROPERTIES

Physical characteristics of bentonite are affected by whether the montmorillonite composing it has water layers of uniform thickness or whether it is a mixture of hydrates with water layers of more than one thickness. Loss of absorbed water from between the silicate sheets takes place at relatively low temperatures (100 - 200°C). Loss of structural water (i.e., the hydroxyls) begins at 450 - 500°C and is complete at 600 - 750°C. Further heating to 800 - 900°C disintegrates the crystal lattice and produces a variety of phases, such as mullite, cristobalite and cordierite, depending on initial

composition and structure. The ability of montmorillonite to rapidly take up water and expand is lost after heating to a critical temperature, which ranges from 105 to 390°C, depending on the composition of the exchangeable cations. The ability to take up water affects the utilisation and commercial value of bentonite).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for bentonite.

Based on an assessment of environmental hazards, NICNAS identified bentonite as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

As a naturally-occurring clay material biodegradation, bioaccumulation and absorption not relevant for this substance.

B. Biodegradation

As an inorganic substance, bentonite will not biodegrade.

C. Environmental Distribution

<u>Adsorption/desorption</u>

Adsorption and desorption are not relevant for naturally occurring clay materials**.**

D. Bioaccumulation

As a naturally occurring inorganic clay material, bentonite is not bioaccumulative.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

As a naturally-occurring clay material, aquatic toxicity is not a relevant property.

B. Aquatic Toxicity

Acute Studies

No data are available regarding the acute toxicity of this substance.

Chronic Studies

No data are available regarding chronic toxicity of this substance.

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Bentonite is a naturally occurring inorganic material. Thus, biodegradation is not applicable to this substance. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to bentonite.

Bentonite is a naturally inorganic substance. Thus, bentonite does not meet the screening criteria for bioaccumulation.

As a naturally occurring clay material, the substance is not expected to be acutely or chronically toxic.

Thus, bentonite is not a PBT substance.**Other Characteristics of Concern**

No other characteristics of concern were identified for bentonite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Bentonite	1302-78-9	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2017). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
meq/g	milliequivalents per gram
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

BUT-2-ENEDIOIC ACID (FUMARIC ACID)

This dossier on but-2-enedioic acid (fumaric acid) presents the most critical studies pertinent to the risk assessment of this substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – But-2-enedioic acid is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Fumaric acid is a white solid organic compound occurring widely in nature. It has a fruit-like taste and has been used as a food additive. Fumaric acid is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil. Fumaric acid is of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): but-2-enedioic acid

CAS RN: 110-17-8

Molecular formula: $C_4H_4O_4$

Molecular weight: 116.07 g/mol

Synonyms: fumaric acid, 2-Butenedioic acid, trans-Butenedioic acid, Allomaleic acid, Boletic acid, (2E)-but-2-enedioic acid, Lichenic acid

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Fumaric Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless crystalline solid	2	ECHA
Melting Point	287°C @ 101.3 kPa	2	ECHA
Boiling Point	Sublimes at 200°C; @ 0.23 kPa, fumaric acid sublimes at 165°C	2	ECHA
Density	1640 kg/m^3 at 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	0.02 Pa @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	-4.02 @ 20°C (Experimental)	2	ECHA
Water Solubility	7 g/L @ 25°C	2	ECHA
Dissociation constant (pKa)	K1= 9.3 x 10^{-4} at 25°C K2= 2.9 x 10^{-5} at 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for fumaric acid.

NICNAS has assessed fumaric acid in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Fumaric acid is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=110-17-8%2C+

B. Partitioning

The pKa of fumaric acid is 3.03 and 4.54, indicating that this substance will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts (PubChem).

Volatilization of fumaric acid from moist soil surfaces is not expected to be an important fate process because the acid exists as an anion and anions do not volatilize (PubChem).

Hydrolysis is not expected to be an important environmental fate process since this substance lacks functional groups that hydrolyze under environmental conditions(PubChem).

C. Biodegradation

The ready biodegradability of fumaric acid was determined using the OECD 301B guideline in a GLP study.

Using a non-adapted sludge from a domestic source the percentage of biodegradation observed comprised 60.1 % after 11 days (i.e. within the 10-d window) and 67.5 % after 28 days. The reference substance (sodium benzoate) incubated under the same conditions showed a percentage biodegradation of 60.1 % after 11 days. Incubation of the test substance and the reference substance demonstrated that the test substance did not significantly inhibit the microbial activity of the activated sludge.

Accordingly, fumaric acid is considered readily biodegradable. [Kl. score = 1]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for fumaric acid. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} values from the molecular connectivity index (MCI) is 0.865 L/Kg. Thus, fumaric acid has a low potential for adsorption to soil and is expected to have very high mobility. Likewise, based on these values along with the fumaric acid's high water solubility, if released to water, it will likely not adsorb to suspended solids or sediments.

E. Bioaccumulation

There are no bioaccumulation studies on fumaric acid. The substance has a low potential for bioaccumulation based on log $K_{ow} \leq 3$.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Fumaric acid is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 presents the results of acute aquatic toxicity studies on fumaric acid.

Table 3 Acute Aquatic Toxicity Studies on Fumaric Acid

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-h LC_{50}	>100	1	ECHA
Daphnia magna	48-h EC_{50}	>100	1	ECHA
Pseudokirchneriella subcapitata	72-h EC_{50}	>100	1	ECHA

Chronic Studies

No data are available.

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Fumaric acid is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Bioaccumulation of fumaric acid is not expected to occur based on it log Kow value of -4.02 (Table 1). Thus, fumaric acid does not meet the screening criteria for bioaccumulation.

No chronic aquatic toxicity data exist on fumaric acid; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Therefore, fumaric acid does not meet the screening criteria for toxicity.

Therefore, fumaric acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for fumaric acid.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
But-2-enedioic acid	110-17-8	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

DoEE. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

U.S. Environmental Protection Agency [EPA] (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
GLP	Good laboratory procedures
HF	Hydraulic Fracturing
IMAP	Inventory Multitiered Assessment and Prioritisation Program

IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
KOCWIN™	USEPA organic carbon partition coefficient estimation model
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
NOEC	no observed effect concentration
OECD	Organisation for Economic and Co-operation Development
Pa	pascal
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USA	United States of America

BUTYL ALCOHOL (1-BUTANOL)

This dossier on butyl alcohol (1-butanol) presents the most critical studies pertinent to the risk assessment of 1-butanol in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997; Kl).

Screening Assessment Conclusion – Butyl alcohol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

n-Butanol or n-butyl alcohol or normal butanol is a primary alcohol with a 4-carbon structure and the chemical formula C_4H_9OH. Its isomers include isobutanol, 2-butanol and tert-butanol. Butanol is one of the group of "fusel alcohols" which have more than two carbon atoms and have significant solubility in water. n-Butanol occurs naturally as a minor product of the fermentation of sugars and other carbohydrates, and is present in many foods and beverages. It is also a permitted artificial flavorant in the United States, used in butter, cream, fruit, rum, whiskey, ice cream and ices, candy, baked goods and cordials. It is also used in a wide range of consumer products.

The largest use of n-butanol is as an industrial intermediate, particularly for the manufacture of butyl acetate (itself an artificial flavorant and industrial solvent). It is a petrochemical, manufactured from propylene and usually used close to the point of manufacture.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Butan-1-ol

CAS RN: 71-36-3

Molecular formula: $C_4H_{10}O$

Molecular weight: 74.123 g/mol

Synonyms: 1-Butanol, 1-Butyl alcohol, 1-hydroxybutane, Butan-1-ol, butyl alcohol, Butyl hydroxide, Butylalcohol, CCS 203, ET5740PTB, Hemostyp, Methylolpropane, n-Butanol, n-Butyl alcohol, N300PTB, Nacol 4, PP100, Propylcarbinol

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of 1-Butanol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear, colourless liquid with an alcoholic odour	-	PubChem
Melting point	<-90°C (pressure not provided)		PubChem
Boiling point	117°C (pressure not provided)		PubChem
Density	810 kg/m^3 @ 20°C		PubChem
Vapour pressure	< 1000 Pa @20°C		PubChem
Partition coefficient (log K_{ow})	1 @ 25°C		PubChem
Water solubility	66 g/L @ 20°C		PubChem
Dissociation Constant (pKa)	16.1 @ 25°C	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for butyl alcohol.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

1-Butanol is readily biodegradable. It is not expected to bioaccumulate and has a low potential for adsorption to soil and sediment.

B. Partitioning

1-Butanol is highly soluble in water. Based upon a Henry's Law constant of 0.893 Pa*m^3/mol, it is expected to volatilise from water and moist soil surfaces. It is also expected to volatilise from dry soil surfaces based upon its vapour pressure. Vapour-phase 1-butanol will be degraded in the

atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 45 hours (PubChem).

C. Biodegradation

1-Butanol is readily biodegradable. In a BOD test, degradation was 87% after 10 days and 92% after 20 days, meeting the 10-day window (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for 1-butanol. Using KOCWIN in EPISuite™ (USEPA, 2019), the estimated K_{oc} value from log K_{ow} of 1.0 is 10.01 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 3.471 L/kg. Based upon these K_{oc} values, if released to soil, 1-butanol is expected to have very high mobility. If released into water, 1-butanol is not expected to adsorb to suspended solids and sediment in water; and, as noted earlier, volatilisation is expected to be an important fate process (PubChem).

E. Bioaccumulation

There are no bioaccumulation studies on 1-butanol. 1-Butanol is not expected to bioaccumulate based on a log K_{ow} of 1.0 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance exhibits a low order of acute and chronic aquatic toxicity as demonstrated by the information provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on 1-butanol.

Table 3 Acute Aquatic Toxicity Studies on 1-Butanol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephelas promelas	96-hour LC_{50}	1,376	1	ECHA
Daphnia magna	48-hour EC_{50}	1,328	1	ECHA
Pseudokirchneriella subcapitata	72-hour EC_{50}	225	1	ECHA

Chronic Studies

The 21-day NOEC from a *Daphnia* reproduction test is 4.1 mg/L (ECHA) [Kl. score = 2].

96-hour EC_{10} to *Pseudokirchneriella subcapitata* is 134 mg/L (ECHA) [Kl. score = 1].

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

1-Butanol is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 1.0, 1-butanol does not meet the screening criteria for bioaccumulation.

The lowest chronic EC_{10} or NOEC value for 1-butanol is >0.1 mg/L. The acute EC_{50} values are >1 mg/L. Thus, 1-butanol does not meet the criteria for toxicity.

The overall conclusion is that 1-butanol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for butyl alcohol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Butyl Alcohol	71-36-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

USEPA. (2019). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre

hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

CALCINED PETROLEUM COKE

This dossier on calcined petroleum coke presents the most critical studies pertinent to the risk assessment of calcined petroleum coke in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the American Petroleum Institute (API) Test Plan and Robust Summaries on Petroleum Coke submitted to the United States Environmental Protection Agency (USEPA) High Production Volume Information System (HPVIS) Chemical Challenge Program (API, 2000; API, 2008). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Calcined petroleum coke is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Calcined petroleum coke is a black-coloured solid produced by the high-pressure thermal decomposition of heavy (high-boiling) petroleum process streams and residues. If released to the environment, petroleum coke is expected to be chemically and physically inert. Calcined petroleum coke is not expected to biodegrade since it is composed mainly of elemental carbon which does not contain the chemical bonds that microbes require for metabolism. Being water-insoluble and physically and biologically inert, calcined petroleum coke is not expected to bioaccumulate. It is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Coke (petroleum), calcined

CAS RN: 64743-05-1

Molecular formula: UVCB (Unknown or Variable Composition, Complex Reaction Products and Biological Materials)

Molecular weight: UVCB

Synonyms: Coke (petroleum), calcined; coke, petroleum, calcined

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Calcined Petroleum Coke

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Black-coloured solid	-	API, 2008; USEPA, 2011
Melting Point	Not applicable	-	API, 2008; USEPA, 2011
Boiling Point	Not applicable	-	API, 2008; USEPA, 2011
Density	700-950 kg/m^3	-	API, 2000

Property	Value	Klimisch score	Reference
Vapour Pressure	Negligible	-	API, 2008; USEPA, 2011
Partition Coefficient (log P_{ow})	Not applicable	-	API, 2008; USEPA, 2011
Water Solubility	Insoluble	-	API, 2008; USEPA, 2011

Petroleum coke consists of two substances: green coke and calcined coke. The principal difference between the substances is the amount of residual hydrocarbon in the two products. Petroleum coke (both green and calcined) is produced by the high-pressure thermal decomposition of heavy (high-boiling) petroleum process streams and residues. Green coke is the initial product from the cracking and carbonisation of the feedstocks to produce a substance with a high carbon-to-hydrogen ratio. Green coke undergoes additional thermal processing to produce calcined coke. The additional processing removes the residual hydrocarbons and increases the percentage of elemental carbon, which results in a lower potential for toxicity (API, 2008).

Green petroleum coke exists as a solid substance composed of predominantly carbon in a polycrystalline porous matrix. Approximately 9-21% by weight of green petroleum coke is volatile matter that is driven off during the calcining process. This volatile matter consists of the heavy hydrocarbons remaining from the feedstocks that have not undergone complete carbonisation. It exists in green coke as a hardened residuum in the carbon matrix. The specific chemical composition of any given batch of petroleum coke is determined by the composition of the feedstocks used in the coking process, which in turn are dependent on the composition of the crude oil and refinery processing from which the feedstock is derived.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for calcined petroleum coke.

NICNAS has assessed calcined petroleum coke in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=64743-05-1

5 ENVIRONMENTAL FATE SUMMARY

Elemental carbon and the residual components are not water-soluble and are not volatile in the environment. The substance is chemically and physically inert. Therefore, biodegradation, atmospheric photooxidation, and hydrolysis will be negligible (USEPA, 2011). Volatilization is negligible. Depending on factors such as particle size and density relationships between the petroleum coke and environmental media, releases to terrestrial or aquatic environments would result in incorporation of the material in soils/sediments or dispersal via wind/water action (API, 2008). While it may be persistent (because not biodegradable), it is not a concern because it has a low environmental or health hazard potential (API, 2000). (API, 2008; USEPA, 2011).

Calcined petroleum coke is not expected to biodegrade since it is composed mainly of elemental carbon which does not contain the chemical bonds that microbes require for metabolism. Other potential constituents embedded in the carbon matrix include inorganic substances and high molecular weight hydrocarbon compounds that may remain as residuum from the coking process. These constituents would not be expected to be available for microbial degradation (API, 2008; USEPA, 2011).

Being water-insoluble and physically and biologically inert, calcined petroleum coke is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Calcined petroleum coke is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Green petroleum coke was tested for potential aquatic toxicity using aqueous exposure solutions prepared as water accommodated fractions (WAFs). An attempt was made to analytically quantify specific organic and inorganic constituents of petroleum coke in the WAF solutions. None of those constituents of petroleum coke were present in the WAF solutions at their analytical detection limits. Because a solubility level could not be established by analytical means, aquatic toxicity test endpoints are presented as nominal WAF loading rates.

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on green petroleum coke.

Table 3 Acute Aquatic Toxicity Studies on Green Petroleum Coke

Test Species	Endpoint	Results (mg/L)*	Klimisch score	Reference
Pimephales promelas	96-hour LL_{50} 96-hour NOELR	>1,000 1,000	1	API, 2008; USEPA, 2011
Daphnia magna	48-hour EL_{50} 48-hour NOELR	>1,000 1,000	1	API, 2008; USEPA, 2011
Selenastrum capricornutum	96-hour EL_{50} 96-hour NOELR	>1,000 1,000	1	API, 2008; USEPA, 2011

*WAF nominal loading rate.

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

Green petroleum coke was tested for potential terrestrial toxicity using aqueous exposure solutions prepared as WAFs (see above text for aquatic toxicity).

The results of acute terrestrial toxicity studies conducted on green petroleum coke are presented in Table 4.

Table 4 Terrestrial Toxicity Tests on Green Petroleum Coke

Test Species	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Earthworm (*Eisenia fetida*)	14-day LC_{50} 14-day NOEC	>1,000 1,000	1	API, 2008; USEPA, 2011
Terrestrial plant (corn)	21-day LC_{50} 21-day NOEC	>1,000 1,000	1	API, 2008; USEPA, 2011
Terrestrial plant (radish)	21-day LC_{50} 21-day NOEC	>1,000 1,000	1	API, 2008; USEPA, 2011
Terrestrial plant (soybean)	21-day LC_{50} 21-day NOEC	>1,000 1,000	1	API, 2008; USEPA, 2011

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Calcined petroleum coke is not biodegradable and thus meets the screening criteria for persistence.

Calcined petroleum coke is not expected to bioaccumulate. Coke is composed of elemental carbon and volatile matter, neither or which are water-soluble and hence not bioavailable. Thus calcined petroleum coke does not meet the screening criteria for bioaccumulation.

No chronic aquatic toxicity studies are available for calcined petroleum coke. However, acute toxicity studies on green petroleum coke showed EC_{50} values of >1,000 mg/L the nominal WAF loading rate. Thus calcined petroleum coke does not meet the screening criteria for toxicity.

The overall conclusion is that calcined petroleum coke is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for calcined petroleum coke.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Calcined Petroleum Coke	64743-05-1	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

American Petroleum Institute (API). (2000). Robust Summary of Information on Petroleum Coke, dated 30 August 2000. Available at: www.petroleumhpv.org.

American Petroleum Institute (API). (2008). Petroleum coke category analysis and hazard characterization. Submitted to the U.S. USEPA by the American Petroleum Institute Petroleum HPV Testing Group, Consortium Registration #1100997, revised August 22, 2008. Available at: www.pet1roleumhpv.org.

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

United States Environmental Protection Agency (USEPA). (2011). Screening-Level Hazard Characterization: Petroleum Coke Category. Sponsored Chemicals: Petroleum coke, green (CASRN 64741-79-3); Petroleum coke, calcined (CASRN 64743-05-1), dated June 2011. Available at: www.petroleumhpv.org.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
API	American Petroleum Institute
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EL	effect level
EU	European Union
HPVIS	High Production Volume Information System
IUPAC	International Union of Pure and Applied Chemistry

kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
LL	lethal loading
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effect concentration
NOELR	No Observed Effect Loading Rate
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction

CALCIUM CARBONATE

This dossier on calcium carbonate presents the most critical studies pertinent to the risk assessment of calcium carbonate in its use in drilling muds and cement additive. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Calcium carbonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Calcium carbonate is an inorganic compound, the most natural forms being chalk, limestone and marble. It is partially soluble in water, dissociating into calcium (Ca^{2+}) and carbonate (CO_3^{2-}) ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. Calcium carbonate is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Calcium Carbonate

CAS RN: 471-34-1

Molecular formula: $CH_2O_3.Ca$ -

Molecular weight: 100.09 g/mol

Synonyms: Carbonic acid, calcium salt (1:1); calcium monocarbonate; monocalcium carbonate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Calcium Carbonate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White powder	1	ECHA
Melting Point	825°C (decomposes) @ 101.3 kPa	2	ECHA
Boiling Point	-	-	-
Density	2700 to 2950 kg/m^3 @ 20 °C	2	ECHA
Vapour Pressure	-	-	-
Partition Coefficient (log K_{ow})	-	-	-
Water Solubility	0.0166 g/L @ 20°C (slightly soluble)	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for calcium carbonate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

"Calcium carbonate, or $CaCO_3$, comprises more than 4% of the earth's crust and is found throughout the world. Its most natural forms are chalk, limestone, and marble, produced by the sedimentation of the shells of small fossilised snails, shellfish, and coral over millions of years."[1]

Calcium carbonate is partially soluble in water, dissociating into calcium (Ca^{2+}) and carbonate (CO_3^{2-}) ions. Both ions are ubiquitous in the environment.

The addition of calcium carbonate to an aquatic ecosystem could result in a shift towards alkalinity and a tendency to increase the pH. The carbonate ions will react with water, forming bicarbonate (HCO_3^-) and hydroxide (OH^-) ions, until an equilibrium is reached. A re-equilibration takes place when carbonate (CO_3^{2-}) is dissolved in water according to the following equations:

$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ $pK_a = 10.33$

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ $pK_a = 6.35$

Only a small fraction of the dissolved CO_2 is present as H_2CO_3 (carbonic acid); the major part is present as CO_2. The amount of CO_2 in water is in equilibrium with the partial pressure of CO_2 in the atmosphere. The CO_2/ HCO_3^-/ CO_3^{2-} equilibria are the major buffers of the pH of freshwater.

Based on these equations, CO_2 is the predominant species at a pH smaller than 6.35, while HCO_3^- is the predominant species at a pH in the range of 6.35-10.33 and CO_3^{2-} is the predominant species at a pH higher than 10.33.

[1] (http://www.ima-na.org/page/what_is_calcium_carb).

Ca^{2+} and CO_3^{2-} ions are not expected to adsorb on particulate matter or surfaces and will not accumulate in living tissues.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Calcium carbonate is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on calcium carbonate.

Table 3 Acute Aquatic Toxicity Studies on Calcium Carbonate (Nano)*

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	>100% (saturated solution)	1	ECHA
Daphnia magna	48-hour EC_{50}	>100% (saturated solution)	1	ECHA
Desmodescus subspicatus	72-hour EC_{50} 72-hour EC_{10}	>14 mg/L** >14 mg/L**	1	ECHA

*The nano form was tested because this form was anticipated to represent the worst case as it was likely to be more soluble than the bulk form due to the smaller particle size and hence greater surface area.
**Highest attainable test concentration that could be prepared due to the limited solubility of the test material.

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

Table 4 lists the results of terrestrial toxicity studies conducted on calcium carbonate.

Table 4 Terrestrial Toxicity Studies on Calcium Carbonate (Nano)*

Test Species	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Eisenia foetida	14-day LC_{50} NOEC	>1,000 1000	1	ECHA
Nitrogen transformation	28-day EC_{50} NOEC	>1,000 1,000	1	ECHA

*The nano form was tested because this form was anticipated to represent the worst case as it was likely to be more soluble than the bulk form due to the smaller particle size and hence greater surface area.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Calcium carbonate is an organic salt that dissociates completely to calcium and carbonate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both calcium and carbonate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Calcium and carbonate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Thus calcium carbonate is not expected to bioaccumulate.

No chronic aquatic toxicity data exist on calcium carbonate; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Thus calcium carbonate does not meet the screening criteria for toxicity.

The overall conclusion is that calcium carbonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for calcium carbonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Calcium Carbonate	471-34-1	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

CALCIUM CHLORIDE

This dossier on calcium chloride presents the most critical studies pertinent to the risk assessment of calcium chloride in its use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA) and the OECD-SIDS documents on calcium chloride (OECD, 2002). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Calcium chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Calcium chloride dissociates completely in aqueous solutions to calcium (Ca2+) and chloride (Cl-) ions. Calcium chloride and its dissociated ions are ubiquitous in the environment. Because of its dissociation properties and high water solubility, calcium chloride is not expected to be adsorbed to soil. Calcium (Ca2+) and chloride (Cl-) ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Neither calcium chloride nor its dissociated ions are expected to bioaccumulate.. Calcium chloride is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Calcium dichloride

CAS RN: 10043-52-4

Molecular formula: $CaCl_2$

Molecular weight: 110.98 gm/mol

Synonyms: Calcium chloride; calcium dichloride; calcium chloride anhydrous

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Calcium Chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White odourless solid; crystals; powder; or granules	2	ECHA
Melting Point	782°C	2	ECHA
Boiling Point	>1,600 °C	2	ECHA
Density	2150 kg/m^3 @ 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	-	-	-
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	745 g/L @ 20°C (very soluble)	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for calcium chloride.

Based on an assessment of environmental hazards, NICNAS identified calcium chloride as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Calcium chloride dissociates completely in aqueous solutions to calcium (Ca^{2+}) and chloride (Cl^-) ions. Calcium chloride and its dissociated ions are ubiquitous in the environment.

Because of its dissociation properties and high water solubility, calcium chloride is not expected to be adsorbed to soil. The calcium ion may bind to soil particulate or may form stable inorganic salts with sulfate and carbonate ions. The chloride ion is mobile in soil and eventually drains into the surface water because it is readily dissolved in water (OECD, 2002).

Calcium (Ca^{2+}) and chloride (Cl^-) ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated (Ganong, 1995). Neither calcium chloride nor its dissociated ions are expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Calcium chloride is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on calcium chloride.

Table 3 Acute Aquatic Toxicity Studies on Calcium Chloride

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	4,630	2	OECD, 2002; ECHA
Lepomis macrochirus	96-hour LC_{50}	9,500-11,300	2	OECD, 2002; ECHA
Gambusia affinis	96-hour LC_{50}	13,400	2	OECD, 2002; ECHA
Lepomis macrochirus	96-hour LC_{50}	10,650	2	OECD 2002; ECHA
Daphnia magna	48-hour EC_{50}	2,400	1	OECD, 2002; ECHA
Daphnia magna	48-hour EC_{50}	2,770	2	OECD, 2002; ECHA
Ceriodaphnia dubia	48-hour EC_{50}	1,830	2	OECD, 2002; ECHA
Daphnia magna	48-hour EC_{50}	1,062	2	OECD, 2002; ECHA
Pseudokirchneriella subcapitata	72-hour EC_{50}	2,900 (biomass)	1	OECD, 2002; ECHA

Chronic Studies

The 21-day EC_{50} and EC_{16} values for calcium chloride in a chronic *Daphnia* reproduction study were 610 and 320 mg/L, respectively (OECD, 2002).

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTIC OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Calcium chloride is an inorganic salt that dissociates completely to calcium and chloride ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both calcium and

chloride ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Calcium and chloride ions are essential to all living organisms, and their intracellular, and extracellular concentrations are actively regulated. Thus, calcium chloride is not expected to bioaccumulate.

A chronic toxicity has been conducted on calcium chloride, but an NOEC of EC_{10} was not determined. The acute EC_{50} values for calcium chloride are >1 mg/L in fish, invertebrates and algae. Thus, calcium chloride does not meet the screening criteria for toxicity.

The overall conclusion is that calcium chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for calcium chloride.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Calcium Chloride	10043-52-4	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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Ganong, W.F. (1995). Review of Medical Physiology, 17th Edition, Appleton & Lange, Norwalk, Connecticut, USA.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2017). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

OECD. (2002). OECD-SIDS: Calcium chloride (CAS No. 10043-52-4), UNEP Publications. Available at: http://www.inchem.org/documents/sids/sids/10043524.pdf

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal

LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

CALCIUM LIGNOSULFONATE

This dossier on calcium lignosulfonate presents the most critical studies pertinent to use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Calcium lignosulfonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Lignin is the second largest component of wood. It is a highly polymerised material that makes up the middle lamella of woody fibres and holds the fibres together. The basic units of the polymeric structure consist of three aromatic propenyl alcohols (monolignols): coniferyl alcohol (4-(3-hydroxy-1-propenyl)-2-methoxyphenol); p-coumaryl alcohol (4-[(E)-3-hydroxyprop-1-enyl]phenol); and sinapyl alcohol (4-hydroxy-3,5-dimethoxycinnamyl alcohol). Coniferyl alcohol represents the principle unit in lignin.

Calcium lignosulfonate is obtained from the spent sulfite and sulfate pulping liquor of wood or from the sulfate (kraft) pulping process. It may contain up to 30% reducing sugars.

This dossier contains toxicity data on calcium lignosulfonate (40-65). Calcium lignosulfonate (40-65) is produced from softwood in the sulfite pulping method for manufacturing paper. In this process, bisulfite ions react with the native lignin polymer of the wood to form sulfonated lignin (lignosulfonate). This reaction increases the water solubility of the hydrophobic lignin polymer. Calcium lignosulfonate contains <5% reducing sugars. The calcium bisulfite provides the calcium ions that stabilise the anionic sulfonate groups in the lignosulfonates. The average molecular weight is in the range of 40,000 to 65,000 daltons, with >90% ranging from 1,000 to 250,000 (EFSA, 2010). Calcium lignosulfonate (40-65) is of higher purity than calcium lignosulfonate, with a higher degree of polymerisation and lower content of sugars.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Calcium lignosulfonate

CAS RN: 8061-52-7

Molecular formula: Not applicable.

Molecular weight: Unknown

Synonyms: Calcium lignosulfonate; lignosulfonic acid, calcium salt; lignin calcium sulfonate

3 PHYSICO-CHEMICAL PROPERTIES

Calcium lignosulfonate and calcium lignosulfonate (40-65) occur as a brown, amorphous polymer (EFSA, 2010). They are soluble in water, but not in any of the common organic solvents.

The pH of a 1:100 aqueous solution of calcium lignosulfonate is between ca. 3 and 11 (EFSA, 2010).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for calcium lignosulfonate.

NICNAS has assessed calcium lignosulfonate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No specific data could be located on the environmental fate/transport of calcium lignosulfonate. The United States Environmental Protection Agency (USEPA) reviewed the environmental fate and environmental hazards of various lignosulfonate chemicals, including sodium lignosulfonate, for a proposed rule to establish 44 tolerance exemptions for residues of these substances (FR, 2005). The USEPA determined "that the various salts of lignosulfonic acid are soluble to very highly water soluble depending on the cation. Once in water dissociation of the cation is expected depending on pH. These lignosulfonates are not expected to be mobile in terrestrial environments, moving equally with the water and sediment phase to surface water. Ground water migration is not likely. Once in water, the dissociated cation and anion are likely to remain in dissolution. The available information suggest that lignosulfonates may be persistent in aquatic environment of low microbial activity and much less persistent in environments with ample microbial activity…though the time for complete aerobic degradation is predicted to be months, the lignosulfonates are strongly absorbed to soils and sediments due to their high-molecular weights." Based on the USEPA assessment, it is concluded that sodium lignosulfonate would meet the EU screening criteria for persistence.

Due to its high-molecular weight, sodium lignosulfonate is not expected to be bioavailable. This is supported by pharmacokinetic data on calcium lignosulfonate which showed that it is poorly absorbed from the gastrointestinal tract of rats (Beck and Rossi, 2005). Thus, it is not expected to bioaccumulate.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=8061-52-7%2C+

6 ENVIRONMENTAL EFFECTS SUMMARY

Because of the lack of data, the EFSA Panel on Additives and Products or Substances used in Animal Feed (FEEDAP) could not conclude on the safety of calcium lignosulfonate for the environment (EFSA, 2015).

A. Aquatic Toxicity

No data are available.

B. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Based on the assessment by the USEPA (FR, 2005), calcium lignosulfonate meets the criteria for persistence.

Calcium lignosulfonate is not expected to bioaccumulate due to its low potential for bioavailability because of its molecular weight and size. Thus, it does not meet the criteria for bioaccumulation.

No aquatic toxicity studies are available for calcium lignosulfonate. It is expected to be a low concern of toxicity to aquatic organisms because of its low potential for bioavailability.

The overall conclusion is calcium lignosulfonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for calcium lignosulfonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Calcium lignosulfonate	8061-52-7	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Beck, M., and Rossi, B. (2005). Absorption, distribution and excretion of tritium labeled lignosulfonate after single oral administration to rats. Report No. 2500147, DSM Nutritional Products Ltd.; cited in EFSA (2010).

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

EFSA [European Food Safety Authority]. (2010). Scientific Opinion on the use of calcium lignosulfonate (40-65) as a carrier for vitamins and carotenoids. EFSA Journal 8(3): 1525. Available at: https://efsa.onlinelibrary.wiley.com/doi/epdf/10.2903/j.efsa.2010.1525.

EFSA. (2015). Scientific Opinion on the safety and efficacy of lignosulphonate as a feed additive for all animal species. EFSA Journal 2105; 13(7):4160. Available at: https://efsa.onlinelibrary.wiley.com/doi/pdf/10.2903/j.efsa.2015.4160

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

FR [Federal Register]. (2005). Lignosulfonates; Exemptions from the Requirement of a Tolerance, 70 Federal Register 7912-7921, February 16, 2005.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EFSA	European Food Safety Authority
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
Kl	Klimisch scoring system
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

CALCIUM OXIDE
CALCIUM HYDROXIDE

This dossier on calcium oxide and calcium hydroxide presents the most critical studies pertinent to the risk assessment of these substances in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Calcium oxide and calcium hydroxide are classified as a **tier 1** chemicals and requires a hazard assessment only.

1 BACKGROUND

Calcium oxide and calcium hydroxide are inorganic compounds. They are partially soluble in water, dissociating into calcium (Ca^{2+}) and hydroxyl (OH^-) ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. The substances are of low toxicity concern to aquatic and terrestrial organisms.

For the purposes of this dossier, information will be focused on calcium oxide as both the oxides and hydroxides of calcium have the same environmental fate and toxicity profiles.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Calcium oxide

CAS RN: 1305-78-8

Molecular formula: CaO

Molecular weight: 56.08 g/mol

Synonyms: Lime; Quicklime; Burnt lime; Calcia; Calxyl; Gebrannter kalk; Unslaked lime; Calcium monoxide

Chemical Name (IUPAC): Calcium dihydroxide

CAS RN: 1305-62-0

Molecular formula: CaH_2O_2

Molecular weight: 74.09 g/mol

Synonyms: calcium hydroxide; slaked lime; hydrated lime; calcium hydroxide, hydrated

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Calcium Oxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid powder - Beige	1	ECHA
Melting Point	> 450°C (pressure not provided)	1	ECHA
Boiling Point	2,850°C @ 101.3 kPa	1	ECHA
Density	3310 kg/m^3 @ 22°C	1	ECHA
Vapour Pressure	-	-	-
Partition Coefficient (log K_{ow})	-	-	-
Water Solubility	1.338 g/L @ 20 °C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for calcium oxide.

Based on an assessment of environmental hazards, NICNAS identified calcium oxide as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

As an inorganic substance, calcium oxide is expected to disassociate in the environment to its respective cation and anion as limited by its aqueous solubility and pH.

In soil as well as in sediment-water systems, calcium oxide will react and release calcium ions and hydroxyl ions. Therefore, relevant information on adsorption/desorption of calcium oxide can be broadened to data on adsorption/desorption of calcium and magnesium. The behaviour of hydroxyl ions depends on the pH buffer capacity of the tested medium. The pH buffer capacity is controlled by a whole range of processes (mineral dissolution/precipitation, protonation/deprotonation of pH dependent charge sites, reaction with CO_2, biological processes, etc.) and as such, partition coefficients are not relevant for the fate and behaviour of OH- in soils or sediment.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Calcium oxide is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on calcium oxide.

Table 3 Acute Aquatic Toxicity Studies on Calcium Oxide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	50.6 mg/L	1	ECHA
Daphnia magna	48-hour EC_{50}	49.1 mg/L	1	ECHA
Pseudokirchneriella subcapitata	72 hour EC_{10}	79.22 mg/L	1	ECHA

Chronic Studies

A 42-day *Oncorhynchus mykiss* test showed that enhanced Ca^{2+} diets (60 mg Ca^{2+}) had no effects on survival. Mean fish weights remained constant across all treatments (ECHA) [Kl Score = 4]. A 14-day *Crangon septemspinosa* test showed an EC_{10} of 32 mg/L (ECHA) [Kl Score = 2].

C. Terrestrial Toxicity

Table 4 lists the results of terrestrial toxicity studies conducted on calcium oxide.

Table 4 Terrestrial Toxicity Studies on Calcium Oxide

Test Species	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Eisenia foetida	14-day LC_{50} NOEC	> 5 000	1	ECHA

Studies on other terrestrial organisms are available and these either do not show effects, or do show effects but at levels which are significantly higher than the PEC values in the chemical safety report. Since the CSA shows that there is no risk for the soil compartment, there is no indication for this test to be conducted. This is in accordance with column 2 of REACH Annex VII.

Calcium and hydroxyl ions are ubiquitous in the environment and are found naturally in soil, water and sediment. Calcium is an important constituent of most soils and the minerals found in soil are mostly compounds of calcium with other substances. Therefore, the performance of long term toxicity tests on terrestrial arthropods is scientifically unjustified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Calcium oxide is an organic salt that dissociates to calcium and hydroxyl ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both calcium and hydroxyl ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Both chronic and acute aquatic toxicity data are >1 mg/L. Thus, calcium oxide does not meet the screening criteria for toxicity.

The overall conclusion is that calcium oxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for calcium oxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Calcium oxide	1305-78-8	Not a PBT	No	No	NA	No	No	No	1	1	1
Calcium hydroxide	1305-62-0	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
PEC	Predicted exposure concentrations
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SGG	Synthetic Greenhouse Gases

CELLOPHANE

This dossier on cellophane presents the most critical studies pertinent to the risk assessment of its use in drilling muds and as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Cellophane is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Cellophane is a thin, transparent sheet made of regenerated cellulose. Its low permeability to air, oils, greases, bacteria and water makes it useful for food packaging. Cellophane is highly permeable to water vapour, but may be coated with nitrocellulose lacquer to prevent this. As well as food packaging, cellophane is used in transparent pressure-sensitive tape, tubing and many other similar applications. Unlike many other similar materials, cellophane is biodegradable.

Cellophane is produced from cellulose from wood, cotton, hemp or other sources. It is dissolved in alkali and carbon disulfide to make a solution called viscose, which is then extruded through a slit into a bath of dilute sulfuric acid and sodium sulfate to reconvert the viscose into cellulose. The film is then passed through several more baths, one to remove sulfur, one to bleach the film, and one to add softening materials such as glycerin to prevent the film from becoming brittle.

A similar process, using a hole (a spinneret) instead of a slit, is used to make a fibre called rayon. Chemically, cellophane, rayon and cellulose are polymers of glucose; they differ structurally rather than chemically. "Cellophane" is a generic term in some countries, while in other countries it is a registered trademark.[1]

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): diiron(3+) trioxidandiide

CAS RN: 9005-81-6

Molecular formula: Unspecified

Molecular weight: Unspecified

Synonyms: None

[1] Background information as cited in Wikipedia (https://en.wikipedia.org/wiki/Cellophane#Material_properties) and referenced from USEPA U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/DTXSID8050491 (accessed March 03, 2021), Cellophane

3 PHYSICO-CHEMICAL PROPERTIES

Cellophane is a polymeric cellulose film. Cellulosic separators in batteries such as cellophane offer the benefits of very small pore sizes, but are not stable in the oxygen atmosphere that results from charging the cell (Cairns, 2009). The density of cellophane is equal to 1,420 kg/m³ (NIST). Cellophane is transparent, strong, flexible and highly resistant to grease, oil and air. The base cellulose film is modified by softeners, flame-resisting materials and dyes, also by coating with other materials. On exposure to heat the untreated film loses strength at 149°C, decomposes at 176-204°C, does not melt, burns readily and is not self-extinguishing (Miles and Briston, 1965).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for cellophane.

NICNAS has assessed cellulose (CAS No. 9004-34-6) in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[2] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Cellophane, as a cellulosic polymer, is expected to degrade in the environment. It is largely transparent to UV light, but prolonged exposure to sunlight weakens viscose rayon fibers. A 6-hour exposure of unstabilized viscose to UV light leads to a loss in in strength of about 4% (McKeen, 2019).

Its polymeric nature precludes bioaccumulation, biomagnification and sorption to sediments or soils. It is not expected to pose a toxicological hazard to environmental receptors.

[2] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9004-34-6

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Cellophane is expected to be of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

No acute toxicity studies are available.

Chronic Studies

No chronic toxicity studies are available.

C. Terrestrial Toxicity

No terrestrial toxicity studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Cellophane is an organic polymer that is likely to degrade over time. For the purposes of this PBT assessment, cellophane is not considered persistent criteria and therefore, the persistent criteria are not met.

Cellophane is not expected to be bioaccumulative or bioconcentrate and therefore does not meet the criteria for bioaccumulation.

Cellophane is not expected to be of a substantial toxicological concern to environmental receptors. Thus, cellophane does not meet the screening criteria for toxicity.

The overall conclusion is that cellophane is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for cellophane.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cellophane	9005-81-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

McKeen, Laurence W. (2019). Chapter 13: Renewable Resource, Sustainable and Biodegradable Polymers. The Effect of UV Light and Weather on Plastics and Elastomers (Fourth Edition),William Andrew Publishing, 2019, Pages 425-438.

Miles DC and Briston JH. (1965). Polymer technology. New York : Chemical Publishing Co. Inc. 444 p.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

CELLULASE ENZYME

This dossier on cellulase enzyme presents the most critical studies pertinent to the risk assessment of cellulase enzyme in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Cellulase enzyme is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Cellulase enzymes are catalytic proteins or polypeptides that consist of amino acids coupled via peptide bonds. Cellulase enzymes cleave ß-1,4-glycosidic bonds in cellulose. Cellulases are readily biodegradable; they are not expected to bioaccumulate or adsorb to soil. Cellulase enzyme has a moderate acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1,4-(1,3;1,4)-β-D-glucan-4-glucanohydrolase

CAS RN: 9012-54-8

Molecular weight: 20,000 to 80,000 Daltons

Synonyms: Cellulase; 1,4-(1,3;1,4)-β-D-glucan-4-glucanohydrolase;

Enzymes are catalytic proteins or polypeptides that consist of amino acids coupled via peptide bonds. There is a broad range of cellulases used commercially that come from fungal and bacterial origins; all are characterised by ß-1,4-endoglucanase activity. Cellulase enzymes cleave ß-1,4-glycosidic bonds in cellulose.

Enzyme preparations are characterised by their enzymatic activity according to the specific methods of the producer. To compare different enzyme preparations, the amount of active substance is normally calculated from the activity via the specific activity of the enzyme, where the protein is determined by active site titration and/or quantitative and qualitative amino acid analysis. The resulting active enzyme protein (aep) content represents a value based on a theoretical pure and totally active enzyme (HERA, 2005).

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Cellulase

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	As pure enzyme, white crystals or powder	-	HERA, 2005

Property	Value	Klimisch score	Reference
Melting Point	Not feasible	-	ECHA
Boiling Point	Not feasible	-	ECHA
Density	>1330 - <1420 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	0.00344 Pa @ 25°C (mean value)	1	ECHA
Partition Coefficient (log K_{ow})	< -1.3 @ 20°C*	1	ECHA
Water Solubility	100 g/L @ 25 °C	-	ECHA

*An octanol-water partition coefficient (K_{ow}) for cellulases is not available. Therefore, the log K_{ow} of glucoamylase, which cleaves 1,4–α-D-glycosidic linkages, was referenced.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for cellulase enzyme.

Based on an assessment of environmental hazards, NICNAS identified cellulase enzyme as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Cellulases are readily biodegradable; they are not expected to bioaccumulate or adsorb to soil.

B. Biodegradation

A cellulase enzyme was readily biodegradable in an OECD 301F test. There was ~10% degradation after one day; ~60% after 5 days; and 129% after 28 days (ECHA). [Kl. score = 1]

Three different cellulase enzymes were considered readily biodegradable based on the results of OECD 301C and 301E tests (HERA, 2005) [Kl. scores = 1]. In an OECD 301E test, there was 84% DOC removal of the enzyme Carezyme after 28 days. In another OECD 301E test, there was 92% DOC removal of the enzyme Clazinase® after 28 days. In an OECD 301C test, BOD/COD was 78% after 28 days (HERA, 2005).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

Proteins, such as cellulase enzyme, would not be expected to adsorb to soil. HERA (2005) listed a K_{oc} value of <1.3 for detergent amylases, cellulases, and lipases that was calculated according to the EU Technical Guidance Document (EC, 2003). No further information was provided. If released to water, based on its low K_{oc} and high water solubility values, cellulase is likely to remain in water and not adsorb to sediment. It is also not expected to adsorb to soil, and, has the potential to be highly mobile.

D. Bioaccumulation

No bioaccumulation studies have been conducted on cellulase enzymes. Cellulase enzymes are not expected to bioaccumulate due to their high molecular weight, high water solubility and their low log K_{ow} (log K_{ow} is <-1.3). Moreover, cellulases are rapidly biotransformed in an organism to lower molecular-weight protein fragments by proteolytic enzymes (proteases), and eventually to the basic amino acids by peptidase enzymes.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Cellulase enzyme has a moderate acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 2 lists the results of acute aquatic toxicity studies on cellulase enzyme.

Table 2 Acute Aquatic Toxicity Studies on Cellulase Enzyme

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hr LC_{50}	>100* >52.1**	1	ECHA

Brachydanio rerio	96-hr LC_{50}	330*	4	HERA (2005)
Daphnia magna	48-hr EC_{50}	>100* >52.1**	1	ECHA
Daphnia magna	48-hr EC_{50}	>1,000**	4	HERA (2005)
Daphnia magna	48-hr EC_{50}	1,000**	4	HERA (2005)
Pseudokirchneriella subcapitata	72-hr EC_{50}	>100* >52.1**	1	ECHA
Scenedesmus subspicatus	72-hr EC_{50}	>1,000**	4	HERA (2005)

*Total organic solids.
**Active enzyme protein.

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Cellulase enzyme is readily biodegradable; thus it does not meet the screening criteria for persistence.

Cellulase enzyme has a high molecular weight (20 to 80 kilo Daltons-kD), hydrophilic properties (high water solubility, log K_{ow} <-1.3), and is readily biotransformed in organisms by proteases and peptidases. Thus cellulase enzyme does not meet the screening criteria for bioaccumulation.

There are no chronic toxicity studies on cellulase enzyme. The acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Thus cellulase enzyme does not meet the criteria for toxicity.

The overall conclusion is that cellulase enzyme is not a PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for cellulase enzyme.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cellulase enzyme	9012-54-8	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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HERA. (2005). Human and Environmental Risk Assessment (HERA) on Ingredients of Household Cleaning Products: α-amylase, CAS No. 9000-90-2; Cellulase (β-(1,4)-glucanase), CAS No. 9012-54-8; Lipase, 9001-62-1, 2005. http://www.heraproject.com.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
COD	chemical oxygen demand

DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kD	kilo Daltons
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

CHOLINE CHLORIDE

This dossier on choline chloride presents the most critical studies pertinent to the risk assessment of choline chloride in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on choline chloride (OECD, 2004), and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Choline chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Choline chloride is readily biodegradable. Distribution modelling using Mackay Level 1 shows choline to be distributed completely into water. Choline chloride is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-Hydroxy-N,N,N-trimethylethanaminium chloride

CAS RN: 67-48-1

Molecular formula: $C_5H_{14}NO.Cl$
$C_5H_{14}NO^+$ (choline)

Molecular weight: 139.6 g/mol
104.2 g/mol (choline)

Synonyms: Choline chloride; 2-hydroxy-N,N,N-trimethylethanaminium chloride; trimethyl(2-hydroxyethyl)ammonium chloride; cholinium chloride; 2-hydroxyethyl(trimethyl)azanium chloride

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Choline Chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	White crystalline solid*	2	OECD (2004)
Melting Point	~ 200°C @ 101.3 kPa	1	ECHA
Boiling Point	Decomposition at 305°C @ 101.3 kPa prior to boiling.	2	ECHA

Property	Value	Klimisch score	Reference
Density	70% aq. solution: 1110 kg/m^3@ 20°C	4	OECD (2004)
Vapour Pressure	2287.2 Pa @ 25°C (QSAR)	2	ECHA
Partition Coefficient (log K_{ow})	75% aq. solution: -3.77 @ 25°C	1	ECHA
Water Solubility	Powder containing 50% choline chloride: 650 g/L (temperature unknown)	4	OECD (2004)
Viscosity	75% aq. solution: 26.2 mPa.s @ 20°C; 14.1 mPa.s @ 40°C	1	ECHA

*Choline chloride is a white crystalline solid; it is marketed as an aqueous solution (70-75% w/w in water), which is colourless with an amine-like odour.

Choline chloride is a quaternary amine salt that will dissociate in water into choline ($C_5H_{14}NO^+$) and chloride (Cl^-) ions.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for choline chloride.

Based on an assessment of environmental hazards, NICNAS identified cholide chloride as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Choline chloride is readily biodegradable. Distribution modelling using Mackay Level 1 shows choline to be distributed completely into water. Choline chloride will not adsorb on soil and sediments. It is not expected to bioaccumulate.

B. Partitioning

Choline chloride is highly water soluble and non-volatile. When released to water under typical environmental conditions, the quaternary ammonium salt dissociates to release a positively charged choline ion and a negatively charged chloride ion (OECD, 2004). It is unlikely to partition to the atmosphere based on its low volatility (OECD, 2004).

C. Biodegradation

Choline chloride is readily biodegradable (93% within 14 days) in a MITI-I test (MITI, 1992; OECD, 2004). In another MITI-I test, biodegradation was ≥60%, indicating ready biodegradation (Tunkel *et al.*, 2000; OECD, 2004). A $BOD_5/ThOD_5$ ratio of 75% was obtained in a BOD_5 test performed according to DIN 38409 part 43 (BASF AG, 1984; OECD, 2004). If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for choline. Choline is a quaternary ammonium compound (QAC); these compounds are not included in the training set for the K_{oc} estimation of the QSAR model KOCWIN v. 2.00 in EPISuite™ (USEPA, 2016), and therefore outside the program's prediction domain. A K_{oc} value of 2.3 had been estimated using the older QSAR model PCKOCWIN v. 1.66 (OECD, 2004), indicating a low potential for soil adsorption potential.

Results from Mackay Level I modelling indicate that choline chloride will be distributed completely into water (OECD, 2004).

E. Bioaccumulation

No measured data on bioaccumulation of choline chloride are available. An experimental log K_{ow} is -3.77, which indicates a low potential to accumulate in organisms (OECD, 2004). Bioaccumulation is not expected in aquatic organisms.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Choline chloride is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on choline chloride.

Table 3 Acute Aquatic Toxicity Studies on Choline Chloride

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oryzias latipes	96-hour LC_{50}	>100 (nominal and measured)	1	MOE Japan (1999a); OECD (2004)
Leuciscus idus	96-hour LC_{50}	>10,000*	2	OECD (2004); ECHA
Daphnia magna	48-hour EC_{50}	349 (nominal and measured)	2	MOE Japan (1999a); OECD (2004)
Daphnia magna	48-hour EC_{50}	>500*	2	OECD (2004)
Pseudokirchneriella subcapitata	72-hour EC_{50}	>1,000 (nominal and measured)	1	MOE Japan (1999a); OECD (2004)

*78% aqueous solution of choline chloride.

Chronic Studies

In a 21-day *Daphnia magna* reproduction test, the nominal and measured NOEC was reported to be 30.2 mg/L (MOE Japan, 1999d) [Kl. score = 1].

The NOEC from a 72-hour algae *Pseudokirchneriella subcapitata* study is 30.2 mg/L (MOE Japan, 1999c; OECD, 2004) [Kl. score = 1].

C. Terrestrial Toxicity

No data are available.

Choline is present in all plant and animal cells, mostly in the form of phospholipids (phosphotidylcholine or lecithin, lysophosphatidylcholine, choline plasmalogens and sphingomyelin), which are essential components of membranes (IOM, 2000).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Choline chloride is readily biodegradable and thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -3.77, choline chloride does not meet the criteria for bioaccumulation.

The NOEC values from chronic toxicity studies on choline chloride are >0.1 mg/L. Thus, choline chloride does not meet the criteria for toxicity.

The overall conclusion is that choline chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for choline chloride.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Choline Chloride	67-48-1	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DIN	Deutsches Institut für Normung
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HENRYWIN	EPISuite modelling component to calculate the Henry's Law constant
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre

KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
m^3	cubic metre
mg/L	milligrams per litre
MITI	Japanese Ministry of International Trade and Industry
mPas	millipascal second
OECD	Organisation for Economic Co-operation and Development
Pa m^3/mol	pascal meter squared per gram molecular weight
PBT	Persistent, Bioaccumulative and Toxic
PCKOCWIN	USEPA Episuite modelling component to calculate K_{oc}
QAC	quaternary ammonium compound
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
ThOD	theoretical oxygen demand

CINNAMALDEHYDE

This dossier on cinnamaldehyde presents the most critical studies pertinent to the risk assessment of cinnamaldehyde in its use in coal seam gas activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Cinnamaldehyde was assessed as a tier 1 chemical for acute toxicity in algae and as a tier 2 chemical for acute toxicity in fish and invertebrates. Cinnamaldehyde was assessed as a tier 1 chemical for chronic toxicity in fish and as a tier 2 chemical for chronic toxicity in invertebrates. However, cinnamaldehyde is determined to biodegrade in the environment very quickly suggesting chronic lab data would be less relevant than acute results. Further, since cinnamaldehyde is readily biodegradable in water, it was considered by ECHA to be non- toxic to aquatic fish, invertebrates and algae at environmentally relevant concentrations. As a result, based on preponderance of data and biodegradation information, cinnamaldehyde is classified overall as a **Tier 1** chemical and requires a hazard assessment only

1 BACKGROUND

Cinnamaldehyde is an organic compound. Occurring naturally as predominantly the trans (E) isomer, it gives cinnamon its flavour and odour. It is a phenylpropanoid that is naturally synthesized. This pale yellow, viscous liquid occurs in the bark of cinnamon trees and other species of the genus Cinnamomum. The essential oil of cinnamon bark is about 90% cinnamaldehyde.

The most obvious application for cinnamaldehyde is as flavouring in chewing gum, ice cream, candy, eliquid and beverages. Cinnamaldehyde is also known as a corrosion inhibitor for steel and other ferrous alloys in corrosive fluids. It is believed that this is achieved by polymerization to form a protective film on the metal surface. It can be used in combination with additional components such as dispersing agents, solvents and other surfactants.

Cinnamaldehyde is expected to biodegrade and not expected to bioaccumulate to any significant extent. It has a low potential to adsorb to soil or sediment. Cinnamaldehyde has low chronic toxicity potential to aquatic organisms. Since cinnamaldehyde is readily biodegradable in water, it was considered to be non- toxic to aquatic fish, invertebrates and algae at environmentally relevant concentrations.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): (2E)-3-phenylprop-2-enal

CAS RN: 104-55-2

Molecular formula: C_9H_8O

Molecular weight: 132.16 g/mol

Synonyms: Cinnamaldehyde; (2E)-3-phenylprop-2-enal; 3-phenylacrylaldehyde; cinnamal; (E)-cinnamaldehyde; 3-phenylpropenal; cinnamic aldehyde; phenylacrolein; cinnamylaldehyde; 3-phenyl-2-propenal; trans-cinnamaldehyde; (E)-3-phenylpropenal; (E)-3-phenyl-2-propenal; 3-phenylacrolein; 3-phenyl-2-propenaldehyde; 3-phenyl-2-propen-1-al; acrolein, 3-phenyl-; 2-propenal, 3-phenyl-; 2-propenal, 3-phenyl-, (2E)-

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Cinnamaldehyde

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid	1	ECHA
Melting point	-18°C @ 101.3 kPa	1	ECHA
Boiling point	>250°C @ 96.99 kPa	1	ECHA
Density	1,041 kg/m^3 @ 20°C	1	ECHA
Vapour pressure	3.853 Pa @ 25°C	1	ECHA
Partition coefficient (log K_{ow})	2.107 @ 25°C	1	ECHA
Water solubility	2.11 g/L @ 22°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for cinnamaldehyde.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Cinnamaldehyde is expected to biodegrade and not expected to bioaccumulate to any significant extent. It has a low potential to adsorb to soil or sediment.

B. Partitioning

Cinnamaldehyde is highly soluble in water. Volatilisation from water surfaces or moist soil surfaces is expected to be an important fate process based upon this compound's estimated Henry's Law constant of 0.35 Pa-m^3/mole . However, it is not expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

C. Biodegradation

Cinnamaldehyde is readily biodegradable. In an OECD 301B test, degradation of cinnamaldehyde was 89% after 7 days, 94% after 14 days, and 100% after 28 days, indicating ready biodegradation (ECHA) [Kl. score = 2]. In an OECD 301D test, biodegradation was 24.98% after 5 days. The BOD_5 value was 0.635 mg O_2/mg (ECHA) [Kl. score = 1].

If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for cinnamaldehyde. Using KOCWIN in EPISUITE™ (EPA, 2018), the estimated K_{oc} value from log K_{ow} of 2.107 is 55.82 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 36.82 L/kg. Based on this estimated value, cinnamaldehyde is expected to have very high mobility in soil. If released to water, based on the K_{oc} value and its water solubility, it is also not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on cinnamaldehyde. Cinnamaldehyde is not expected to bioaccumulate based on a log K_{ow} of 2.107 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Cinnamaldehyde has low chronic toxicity potential to aquatic organisms. Since cinnamaldehyde is readily biodegradable in water, it was considered to be non- toxic to aquatic fish, invertebrates and algae at environmentally relevant concentrations.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on cinnamaldehyde.

Table 3 Acute Aquatic Toxicity Studies on Cinnamaldehyde

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio (previous name Brachydanio rerio)	96-hr LC_{50}	> 3.9 <5.5	1	ECHA
Poecilia reticulata (Guppy fish)	96-hr LC_{50}	> 3.5 < 6.5	2	ECHA
Lepomis macrochirus (Bluegill fish)	96-hr LC_{50}	>20	2	ECHA
Daphnia magna	48-hr EC_{50}	3.21	2	ECHA
Daphnia magna	48-hr EC_{50}	3.86	2	ECHA
Daphnia magna	48-hr EC_{50}	11.5	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50}	31.6	2	ECHA
Chlorella vulgaris	72-hr EC_{50}	16.09	2	ECHA

Since the test chemical is readily biodegradable in water, the chemical was considered to be non-toxic to aquatic fish, invertebrates and algae at environmentally relevant concentrations (ECHA).

Chronic Studies

Based on the prediction done using ECOSAR version 1.11, the long term toxicity on fish was predicted for cinnamaldehyde. On the basis of effects observed in a flow through freshwater system on test organism, the NOEC value for the substance was estimated to be 15.159 mg/L for fish for 28 days of exposure duration. (ECHA) [Kl. score = 2].

In an OECD 211 *Daphnia magna* Reproduction Test toxicity study, the 21-day EC_{50} value was 0.402 mg/L. (ECHA) [Kl. score = 2].

C. Terrestrial Toxicity

In a short-term toxicity study to birds (avoidance [repellency] test), the 5-day LOEL value was 1% w/w for *Colinus virginianus* (Northern Bobwhite Quail). (ECHA) [Kl. score = 2].

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Cinnamaldehyde is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 2.107, cinnamaldehyde does not meet the screening criteria for bioaccumulation.

The NOEC from a chronic fish study is >0.1 mg/L. The acute E(L)C_{50} values for cinnamaldehyde are >1 mg/L. Thus, cinnamaldehyde does not meet the criteria for toxicity.

The overall conclusion is that cinnamaldehyde is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for cinnamaldehyde.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cinnamaldehyde	104-55-2	Not a PBT	No	No	No	No	No	No	2 (Fish & Inv), 1 (Algae)	1 (Fish), 2 (Inv)	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). Rapid degradation suggests substance will not reasonably expose environmental receptors to levels of toxicological concern.

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biochemical oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union

g/L	grams per litre
Hg	mercury
IUPAC	International Union of Pure and Applied Chemistry
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kg/m^3	kilograms per cubic metre
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
m^3/mol	cubic metres per mole
MCI	molecular connectivity index
mg	milligrams
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mm	millimetre
mPa s	millipascal second
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

CITRIC ACID

This dossier on citric acid presents the most critical studies pertinent to the risk assessment of citric acid in its use in drilling muds and hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on citric acid (OECD 2001a,b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Citric acid is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Citric acid is readily biodegradable and is not expected to bioaccumulate. Citric acid is a low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-Hydroxy-1,2,3-propanetricarboxylic acid

CAS RN: 77-92-9

Molecular formula: $C_6H_8O_7$

Molecular weight: 192.122 g/mol

Synonyms: citric acid; 1,2,3-propanetricarboxylic acid, 2-hydroxy-; 2-hydroxy-1,2,3-propanetricarboxylic acid

3 PHYSICO-CHEMICAL PROPERITES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Citric Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White crystalline solid; odourless.	2	ECHA
Melting Point	153°C @ 101.3 kPa	2	ECHA
Boiling Point	Not available; decomposition	-	ECHA
Density	1670 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	2.21 x 10^{-6} Pa @ 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-1.61 to -1.80 (temperature not indicated)	2	ECHA
Water Solubility	590 g/L @ 20°C (very soluble)	4	ECHA
Dissociation Constant (pKa)	3.13, 4.76 and 6.4 @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for citric acid.

Based on an assessment of environmental hazards, NICNAS identified citric acid as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Citric acid is readily biodegradable. It is not expected to bioaccumulate. Due to its high water solubility, citric acid is unlikely to adsorb to soil or sediment.

B. Partitioning

The pKa of citric acid varies between 3.13 and 5.4 at 25°C (ECHA). [KI Score = 2]. These values indicate that this compound will exist almost entirely in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil is not expected because the compound exists as an anion and anions do not volatilize. Likewise, citric acid is not expected to volatilize from dry soil surfaces based upon its vapor pressure (PubChem).

C. Biodegradation

Citric acid can be considered readily biodegradable based on the results of the ready and inherent aerobic biodegradation studies listed in Table 3. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

Table 3 Biodegradation Studies on Citric Acid (OECD 2001a,b)

Test System	Results*	Notes	Klimisch Score
Modified Sturm	97% (CO_2 evolution); 100% (DOC removal)	Readily biodegradable; exposure period not stated	2
Closed Bottle Test	BOD_{30}/COD Ratio = 90%	Readily biodegradable	2
BOD_5/COD Ratio	BOD_5 = 526 mg; COD = 728 mg; BOD_5/COD Ratio = 0.72	Readily biodegradable; concentration of test substance and activated sludge not stated	2
BOD_1/ThOD Ratio	BOD_1/ThOD Ratio = 13%	-	2
BOD_{20}/ThOD Ratio	BOD_{20}/ThOD Ratio = 98%	Readily biodegradable; initial test substance concentration 720 mg/L	2
Zahn-Wallen Test	85%, 1 day (DOC removal)	Inherently biodegradable	2
Zahn-Wallen Test	98%, 7 days (DOC removal)	Inherently biodegradable	
Coupled Units Test	93% (COD removal)	Ultimately biodegradable; exposure period not stated.	2

D. Environmental Distribution

No experimental data are available for citric acid. Using KOCWIN program in EPISuite™ (USEPA, 2016), the estimated K_{oc} value from the K_{ow} value of -1.08 is 0.3617 L/kg, which suggests a high mobility in soil.

E. Bioaccumulation

The log K_{ow} for citric acid is -1.61 to -1.80. Thus, citric acid is not expected to bioaccumulate.

6 ENVRIONMENTAL EFFECTS SUMMARY

A. Summary

Citric acid is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

The 48-hour LC_{50} values in *Leuciscus idus melanotus* (golden orfe) from two separate laboratories were 440 mg/L and 760 mg/L (ECHA) [Kl. scores = 2]. The 96-hour LC_{50} in *Lepomis macrochirus* (fathead minnow) is >100 mg/L (ECHA) [Kl. score = 2).

The 24-hour EC_{50} in *Daphnia* is 85 mg/L in un-neutralised test solution and 1,535 mg/L in a neutralised solution (OECD, 2001a,b; ECHA). [Kl. score = 2]

The 8-day toxicity threshold value (EC_0) in *Scenedesmus quadricauda* is 640 mg/L (ECHA; OECD, 2001a,b). [Kl. score = 2]

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARCATERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Citric acid is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The log K_{ow} values for citric acid are -1.61 to -1.80. Thus, citric acid does not meet the screening criteria for bioaccumulation.

There are no adequate chronic aquatic toxicity studies on citric acid. The acute EC_{50} values for citric acid are >1 mg/L in fish and invertebrates. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that citric acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for citric acid.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Citric acid	77-92-9	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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USEPA. (2016). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	Biological oxygen demand

COC	constituent of concern
COD	Chemical oxygen demand
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg	milligram
mg/L	milligrams per litre
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

COFFEE EXTRACT

This dossier on coffee extract presents the most critical studies pertinent to the risk assessment of coffee extract in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Coffee extract is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Coffee extract is inherently biodegradable and is expected to have a low potential for bioaccumulation. The potential for adsorption is unknown; however, the low octanol water partition coefficient for coffee extract suggests that it is low. Coffee extract has a low acute toxicity concern for aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Coffee, bean, roasted, extract

CAS RN: 68916-18-7

Molecular formula: UVCB substance

Molecular weight: UVCB substance

Synonyms: Coffee extract; coffee, bean, roasted, extract

3 PHYSICO-CHEMICAL PROPERITES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Coffee Extract

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Viscous liquid	2	ECHA
Melting point	ca. -16.82 to -15.95°C (pressure not provided)	1	ECHA
Boiling point	>102.21°C (pressure not provided)	1	ECHA
Density	1234 kg/m^3 @ 20°C	1	ECHA
Vapour pressure	21.8 Pa @ 20°C	1	ECHA
Partition coefficient (log K_{ow})	<0.36 @ 25°C	1	ECHA

Property	Value	Klimisch score	Reference
Water solubility	0.00285 g/L @ 25°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for coffee extract.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Coffee extract is inherently biodegradable and is expected to have a low potential for bioaccumulation. The potential for adsorption is unknown; however, the low octanol water partition coefficient for coffee extract suggests that it is low.

B. Biodegradation

Coffee extract is inherently biodegradable. In an OECD 301D test, degradation was 50.2% after 28 days (ECHA) [Kl. score = 1].

C. Environmental Distribution

No experimental data are available for coffee extract. Coffee extract is a UVCB substance containing a wide range of different constituents thus, a K_{oc} value has not been calculated.

D. Bioaccumulation

No bioconcentration studies have been conducted on coffee extract. Coffee extract is not expected to bioaccumulate based on the experimental log K_{ow} of <0.36 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Coffee extract has a low acute toxicity concern for aquatic life.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on coffee extract.

Table 3 Acute Aquatic Toxicity Studies on Coffee Extract

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LL_{50}	>100 WAF	1	ECHA
Daphnia magna	48-hour EL_{50}	>100 WAF	1	ECHA
Pseudokirchneriella subcapitata	72-hour EL_{50}	>100 WAF (growth)	1	ECHA

WAF = water accommodated fraction

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Coffee extract is not readily biodegradable, but it does appear to be inherently biodegradable; thus, it is not expected to meet the screening criteria for persistence.

Based on a measured log K_{ow} of <0.36, coffee extract does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on coffee extract. The acute EL_{50} values for coffee extract are >1 mg/L for fish, invertebrates and algae. Thus, coffee extract does not meet the screening criteria for toxicity.

The overall conclusion is that coffee extract is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for coffee extract.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Coffee, bean, roasted, extract	68916-18-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EL	Effective loading
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
LL	Lethal loading
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction

Crystalline Silica, Quartz
(CAS No. 14808-60-7)

Crystalline Silica, Cristobalite
(CAS No. 14464-46-1)

Crystalline Silica, Tridymite
(CAS No. 15468-32-3)

Non-crystalline Silica (Impurity)
(CAS No. 7631-86-9)

Diatomaceous earth
(CAS No. 61790-53-2)

Diatomaceous earth, calcined
(CAS No. 91053-39-3)

This dossier on crystalline silica, quartz, cristobalite and tridymite; non-crystalline silica (impurity); diatomaceous earth; and, diatomaceous earth, calcined presents the most critical studies pertinent to the risk assessment of these substances in their use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

For the purpose of this dossier, crystalline silica, quartz (CAS No. 14808-60-7) has been reviewed as representative of crystalline silica cristobalite and tridymite, and non-crystalline silica (impurity). Crystalline silica, quartz is also considered representative of diatomaceous earth and diatomaceous earth, calcined, as they both consist mainly of silicon dioxide.

Screening Assessment Conclusion – Crystalline silica, quartz, cristobalite and tridymite; non-cyrstalline silica (impurity); diatomaceous earth; and, diatomaceous earth, calcined are classified as **tier 1** chemicals and require a hazard assessment only.

1 BACKGROUND

Crystalline silica is a common mineral found in the earth's crust. Materials like sand, stone, concrete and mortar contain crystalline silica. It will not biodegrade, bioaccumulate, nor will it sorb to sediments or soils. Crystalline silica is expected to exhibit low acute toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): dioxosilane

CAS RN: 14808-60-7

Molecular formula: SiO_2

Molecular weight: 60.084 g/mol

Synonyms: Cristobalite, Dioxide, Silicon

3 PHYSICO-CHEMICAL PROPERTIES

Silica is an off-white granule that occurs naturally in various crystalline and amorphous or other non-crystalline forms. Crystalline silica is characterised by silicon dioxide (SiO_2) molecules oriented in fixed, periodic patterns to form stable crystals. The primary crystalline form of silica is quartz. Other crystalline forms of silica include cristobalite, tripoli and tridymite. Particle size is a key determinate of silica toxicity, since toxicity is restricted to particles that are small enough to be deposited into the target regions of the respiratory tract.

See attached OECD-SIDS Initial Targeted Assessment Profile on Quartz and Cristobalite, SIAM 32, 19-21 April 2011.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for crystalline silica, quartz.

Based on an assessment of environmental hazards, NICNAS identified members of this group (crystalline silica, quartz, cristobalite and tridymite and diatomaceous earth, calcined) as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Crystalline silica is characterised by silicon dioxide (SiO_2) molecules oriented in fixed, periodic patterns to form stable crystals. The primary crystalline form of silica is quartz. It is a stable solid

under typical environmental conditions. It will not biodegrade, bioaccumulate, nor will it sorb to sediments or soils.

B. Biodegradation

No data are available. Based on the crystalline form of the substance it in not expected to biodegrade.

C. Environmental Distribution

No experimental data are available for crystalline silica. As a stable inorganic solid, it is not soluble in water and it will not sorb to soils or sediment.

D. Bioaccumulation

There are no bioaccumulation studies on crystalline silica.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Although no data are available, crystalline silica is expected to exhibit low acute toxicity to aquatic organisms.

B. Aquatic Toxicity

No aquatic toxicity data were available.

C. Terrestrial Toxicity

No terrestrial toxicity data were available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008a).

Crystalline silica is an inorganic mineral. Thus, biodegradation is not applicable to this substance. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to crystalline silica.

As an inorganic complex it is not expected to bioaccumulate. Thus, crystalline silica does not meet the screening criteria for bioaccumulation.

Crystalline silica is not expected to cause adverse effects in environmental receptors. Thus, this substance does not meet the screening criteria for toxicity.

Therefore, crystalline silica is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for crystalline silica, quartz.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Crystalline silica, quartz	14808-60-7	Not a PBT	No	No	NA	No	No	No	1	1	1
Crystalline Silica, cristobalite	14464-46-1	Not a PBT	No	No	NA	No	No	No	1	1	1
Crystalline silica, tridymite	15468-32-3	Not a PBT	No	No	NA	No	No	No	1	1	1
Non-crystalline silica (impurity)	7631-86-9	Not a PBT	No	No	NA	No	No	No	1	1	1
Diatomaceous earth	61790-53-2	Not a PBT	No	No	NA	No	No	No	1	1	1
Diatomaceous earth, calcined	91053-39-3	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2017). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Appendix

OECD-SIDS Initial Targeted Assessment Profile on Quartz and Cristobalite, SIAM 32, 19-21 April 2011

https://hpvchemicals.oecd.org/ui/handler.axd?id=b68bb357-e6dd-4db9-b05c-8148223fc0ff

INITIAL TARGETED ASSESSMENT PROFILE (Human Health)

<table>
<tr><td>CAS No.</td><td colspan="2">Quartz: CAS RN 14808-60-7

Cristobalite: CAS RN 14464-46-1</td></tr>
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 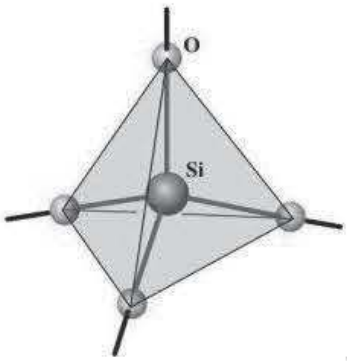
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 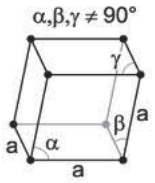

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 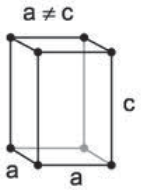

Cristobalite: CAS RN 14464-46-1</td></tr>
</table>

SUMMARY CONCLUSIONS OF THE TARGETED ASSESSMENT

NOTE: The present assessment is targeted to address the following human health endpoints: repeated dose toxicity and carcinogenicity via the inhalation route of exposure, and genotoxicity. It cannot be considered as a full SIDS Initial Assessment. Summary information on exposure is also reported here. Other endpoints for human health and the environment included in the Canadian screening assessment but have not been presented to OECD member countries, and thus are not included in this profile.

The final screening assessment has been published under the responsibility of the Government of Canada. [http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=1EB4F4EF-1].

Rationale for Targeting the Assessment

The Government of Canada "categorized" or prioritized all 23,000 chemical substances on its Domestic Substances List (DSL) from 1999 to September 2006, as required by its *Canadian Environmental Protection Act, 1999* (CEPA 1999). Additional details may be found at http://www.chemicalsubstanceschimiques.gc.ca/about-apropos/categor/index-eng.php. Using information from Canadian industry, academic research and other countries, Government of Canada scientists applied a set of rigorous tools to the 23,000 chemical substances on the DSL. They were categorized to identify those that were: **inherently toxic** to humans or to the environment and that might be **persistent** and/or **bioaccumulative**; and substances to which people might have **greatest potential for exposure**. During this priority-setting exercise, distinct approaches were taken for identifying substances of likely concern for human health and the environment, and subsequent assessment activities may have focused on either human health or ecological

endpoints. Through categorization, the Government of Canada has identified approximately 4,000 of the 23,000 chemical substances on the DSL as priorities for further assessment, research and/or measures to control their use or release. Quartz and cristobalite were identified at that time, applying the categorization criteria, as high priorities for human health risk because they were considered to pose greatest potential for exposure and their respirable forms are classified by the International Agency for Research on Cancer as carcinogenic to humans (quartz and cristobalite) and by the National Toxicology Program as known human carcinogens (crystalline silica). These substances did not meet the ecological categorization criteria for bioaccumulation potential or inherent toxicity to aquatic organisms.

Under the Canadian legislation a determination of whether one or more of the criteria of the CANADIAN ENVIRONMENTAL PROTECTION ACT (CEPA) 1999, section 64 are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and the use of consumer products. A conclusion under CEPA 1999 on the substances in the Chemicals Management Plan (CMP) Challenge is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the Controlled Products Regulations, which is part of the regulatory framework for the Workplace Hazardous Materials Information System [WHMIS] for products intended for workplace use.

Physical-chemical properties

The silicon dioxide group represents a polymorphic category containing a large number of forms identical in composition but with different atomic arrangements which afford different chemical properties. There are two sub-categories within this group: crystalline silica, to which the present substances quartz and cristobalite belong, and non-crystalline or amorphous silica. The key distinction between these sub-categories is that in crystalline substances, the building blocks are arranged in regular, repeating 3-dimensional pattern having long range order, whereas amorphous materials do not display long range order. In all forms of silica, (crystalline and non-crystalline), the silicon atom is tetrahedral and bound to four neighbouring oxygen atoms.

Quartz and cristobalite are solid at room temperature, existing normally as colourless or white crystals. The melting points for quartz and cristobalite are 1400-2000 ^{o}C and 1713-1728 ^{o}C, respectively and for both compounds, the boiling point is 2230^{o}C. Even though no experimental data were available, their vapour pressure and Henry's Law constant are likely negligible. Log K_{ow} (octanol-water partition coefficient) and log K_{oc} (organic carbon-water partition coefficient) are not applicable to these substances. The densities range from 2500-2700 kg/m^3 for quartz and 2300-2380 kg/m^3 for cristobalite.

The very similar physico-chemical properties of quartz and cristobalite reflect their closely related crystal forms. The solubility of crystalline silicates decreases as a function of silica tetrahedral packing density and long-range crystal order. For example, cristobalite has a more open framework structure than quartz and its density is lower, therefore, its solubility is higher. The water solubility of these minerals is also function of temperature, pH, particle size, and the presence of a disrupted surface layer. This may explain the variability of solubility values reported by many authors. The most probable solubility value for quartz is approximately 3.8 mg Si/L, or 6.4 mg/L expressed as the SiO_2 species, while the solubility of cristobalite is approximately 8.7 mg Si/L, or 18 mg SiO_2/L. The kinetics of dissolution of these substances is slow due to the high activation energy required to hydrolyse the Si-O-Si bond.

Human Health Targeted Endpoints

The majority of the studies described here have been reviewed by the International Agency for Research on Cancer (IARC 1997). However, additional data relevant to the screening assessment were identified up to August 2010.

Repeated dose toxicity/non-neoplastic effects (development of silicosis).

Studies on animals

Significant short-term and subchronic studies have demonstrated adverse effects in the lungs, while one of the 6 studies showed effects on the spleen in mice. Rats were exposed to 0, 10 or 100 mg/m^3 of cristobalite via inhalation for 6 hours/day during 3 days. Animals were observed 3 months after exposure. Elevated levels of granulocytes and elevated markers of cytotoxicity from the lung lavage fluid were noted in all exposed groups. Another study of similar duration (9 days) conducted in mice also identified a LOAEC of 10 mg/m^3. Effects observed included minimal interstitial thickening, accumulations of mononuclear cells and slight lymphoid tissue hypertrophy in the lungs.

In a 4-week inhalation study, female rats were exposed to 0, 0.1, 1 or 10 mg/m^3 of quartz 6 hours/day, 5

days/week. Bronchoalveolar lavage fluid was evaluated at 1, 8, and 24 weeks after exposure. Elevated levels of granulocytes and significant elevation of markers of cytotoxicity (Lactate dehydrogenase [LDH] and β-glucuronidase [β-glu]) were observed at 1 mg/m^3 and higher. The increased levels of LDH and β-glu were only significant at 24 weeks after exposure. A LOAEC of 1 mg/m^3 was identified at 24 weeks.

Male rats (4 animals per dose) were exposed to 0 or 3 mg/m^3 of cristobalite via inhalation for 6 hours/day, 5 days/week during 13 weeks. Pulmonary inflammation and fibrosis were observed in the exposed group at the end of treatment. When mice were similarly exposed to 5 mg/m^3 of quartz for 6 hours/day, 5 days/week for 15 or 27 weeks, the authors observed increased spleen weight and formation of plaque in the spleen.

In two separate studies, in which rats or hamsters were exposed to quartz via inhalation for at least 6 months, LOAECs of 2 and 3 mg/m^3 were identified, respectively. All the effects observed were related to inflammation and fibrosis of the lung tissue.

Several chronic studies investigated exposure of the respirable forms (i.e. accumulated via inhalation in the lung tissues) of quartz and cristobalite to rats, mice and hamsters. The following is a description of the study in which the lowest non-neoplastic LOAEC was determined. Groups of 50 rats/sex were exposed 6 hr/day, 5 days/week for 24 months to filtered air or 1 mg/m^3 of DQ-12 quartz, containing 74% of respirable quartz, through whole-body inhalation. An additional 50 rats/sex were exposed to 5 mg/m^3 of titanium dioxide as positive controls. The mean mass of particle at the end of the exposure period was 0.91 mg/lung. The LOAEC identified was 0.74 mg/m^3 (adjusted for 74% respirable quartz) based on lipoproteinosis, multifocal, inflammatory cell infiltrate and alveolar hyperplasia.

Human epidemiology data

In humans, the lowest observed adverse effect level was identified in a U.S. cohort study. The study was conducted on 3330 gold miners (all are males), who had an average of 9 years underground exposure during the period 1940 to 1965. The cohort was followed up through 1990. Silicosis[1] was identified through death certificates or chest X-rays. A job-exposure matrix together with work history was used to estimate individual exposure. The total silica content in the respirable dust in the mine was estimated at 13% and the median crystalline silica exposure was 0.05 mg/m^3. In this sub population of miners, 170 cases of silicosis were identified. The best predictor for risk of silicosis was cumulative exposure, which varied from less than 1% for a 0.5 mg/m^3-year exposure to 68-84% when exposed to more than 4 mg/m^3-year (based on the average daily dust exposure during the workday each year and summed over time for each miner). The main limitations identified

[1] Silicosis: Lung disease caused by inhalation of crystalline silica dust, and resulting in inflammation and scarring in forms of nodular lesions in the upper lobes of the lungs. By definition, clinically or pathologically diagnosed silicosis implies prior exposure to silica (Silicotics). It does not follow that a history of exposure to silica necessarily results in silicosis (Nonsilicotics). The typical "Silicotic" lung nodule is shown in Figure 1.

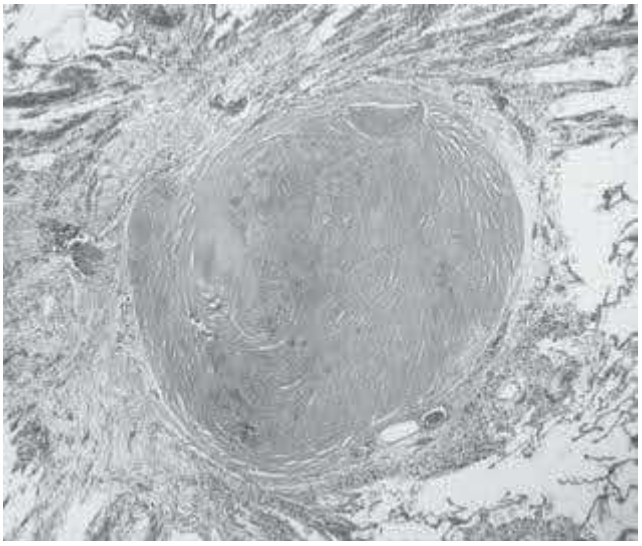

Figure 1. Silicotic nodule characterised by a central zone of hyalinised collagen with a whorled appearance and peripheral dust-containing macrophages (Rees and Murray, 2007).

by the authors include the limited number of radiographic surveys, the potential bias from death certificates (relying on death certificates instead of relying on repeated x-rays, which were lacking for each miner, may have underestimated the number of cases) and the fact that the conversion of dust counts to

gravimetric measurements may not be accurate based on the estimation of 13% silica content in the respirable dust (although based on a relatively large number of samples (n = 82) collected in two different surveys, there was broad range of content in these samples (1% to 48%, SD = 9), and the percentage of respirable quartz may have differed in earlier years, but data were lacking for these years).

Two other human studies have identified similar LOAECs based on the critical endpoint of radiographic confirmed silicosis. A LOAEC of 0.053 mg/m^3 (mean exposure) was identified in a cross sectional study of South African gold miners and a LOAEC of 0.064 mg/m^3 (mean exposure) was derived in a mining community population-based random sample survey in Colorado.

Carcinogenicity studies

Studies on animals

Experimental studies conducted in rats have shown clear and consistent increases in lung tumours after chronic inhalation exposure. In the nine rat studies identified, five were inhalation studies and four were intratracheal instillation studies. All studies except one inhalation study showed increased incidence of lung tumours. For the inhalation studies with treatment related tumours, concentrations ranged from 1 to 50 mg/m^3 (1, 6, and 30 mg/m^3 of DQ-12 quartz; 12 and 50 mg/m^3 of Min-U-Sil 5 quartz) and duration of exposure ranged from 29 days to 2 years. In the inhalation study with no treatment-related tumours, exposure was 60 mg/m^3 of Sikron F300 quartz for 13 weeks. The following is a description of the neoplastic results in the study also identified as the critical study for non-neoplastic results. Groups of 50 rats/sex were exposed 6 hr/day, 5 days/week for 24 months to filtered air or 1 mg/m^3 of DQ-12 quartz through whole-body inhalation. An additional 50 rats/sex were exposed to 5 mg/m^3 of titanium dioxide as positive controls. In the exposed group, 18 animals developed tumours (12 in females, 5 in males), as opposed to 3 and 2 for the control and positive control groups respectively. The majority (10/18) of the tumours observed were adenocarcinomas. The mean mass of particles in the lungs at the end of the exposure period was 0.91 mg/lung.

For the intratracheal instillation studies, doses ranged from 4 to 57 mg/kg-bw (based on 7, 12 or 20 mg/animal of Min-U-Sil (5) quartz or 20 mg/animal of novaculite quartz). Exposure regimes were diverse and included single instillation with observation for up to two years, to weekly instillation for 10 weeks. It is noteworthy that the single intratracheal administration of a 95% pure quartz particles (<5 μm) resulted in an increased incidence of silicotic granulomas after 3 weeks and lung tumours after 11 months. The most common tumours reported across the long term rat studies were adenocarcinomas, however other tumours such as squamous-cell carcinoma, alveolar carcinoma and bronchiole-alveolar adenoma were also reported, and all animals that developed tumours also showed some degree of fibrosis.

Of particular interest is the intratracheal instillation study, investigating the sequence of pathological events leading to lung tumors. An unspecified number of rats/sex/dose received a single intratracheal instillation of various crystalline silica dusts or ferric oxide, allowing direct administration into the bronchial tree. The doses were 12 or 20 mg of Min-U-Sil 5 quartz (MQZ), 12 mg of hydrofluoric-acid-etched Min-U-Sil 5 quartz (HFMQZ), 12 mg of cristobalite, 12 mg of tridymite and 12 mg of ferric oxide suspended in saline. All groups were observed until six months post exposure, except for both MQZ groups, the HFMQZ and the ferric oxide group which were observed up until 17 months post-exposure. Interim sacrifices were conducted at 6, 11 and 17 months. The rat lungs showed a clear progression of effects. The sequence of pathological events were, an initial inflammatory response leading to a marked hyperplasia and hypertrophy of alveolar cells after one month, and at six months hyperplasia was evident but no lung tumours were observed. In this study, lung tumours were observed starting at the 11 month sacrifice with a 17% and 42% incidence in males and females (based on 3/18 males and 8/19 females), respectively, and at 17 months incidences were 32% and 59% (based on 6/19 males and 10/17 females, respectively). No lung tumours were found in ferric oxide treated rats. Similar studies have also been conducted in hamsters and mice. Although treated mice and hamsters showed treatment related signs (inflammation or fibrosis), no tumours were observed in hamsters. No increase in the incidence of lung tumours was seen in mice treated with quartz; however silicotic granulomas and lymphoid cuffing around airways but no fibrosis were seen in the lungs of quartz-treated mice.

Human epidemiology data

There is an extensive dataset of human studies investigating the link between crystalline silica exposure and cancer. IARC (1997) identified over 50 epidemiological studies based on occupational exposure to dust containing respirable crystalline silica. Main industry sectors from which the human data is derived include gold mines, foundries, granite/stone industry, pottery workers and refractory brick workers. From the least

confounded studies, it was noted that lung cancer tended to increase with the following parameters: cumulative exposure; duration of exposure; peak intensity of exposure; presence of radiographically defined silicosis; and length of follow-up time from date of silicosis diagnostic. By definition, clinically or pathologically diagnosed silicosis implies prior exposure to silica (Silicotics).

Since the 1997 IARC report, a large number of epidemiological studies have been published, with the more recent studies being updates from supplementary follow-up of results from previously assessed case-control studies cohorts, new results based on refined exposure assessments or adjustment for confounders or meta-analyses of the pooled data from these epidemiology studies

In a meta-analysis of the data from 10 cohort studies of gold, tin and tungsten miners, granite workers, industrial sand, diatomaceous earth and pottery workers with quantitative exposure estimates for crystalline silica were pooled in order to analyse the risk related to lung cancer. The pooled cohort standardized mortality ratio (SMR, against national rates) [See Appendix 1 for definition] was 1.2 (Confidence Interval [CI] 1.1-1.3). The results from the case-control analyses show a statistically significant trend with duration of exposure (odds ratios (ORs) [See Appendix 1] by quintile of cumulative exposure increased from 1.0 to 1.6 [CIs of 0.85 to 2.1] and by quintile of average concentration increased from 1.0 to 1.7 [CIs of 1.1 to 2.3]), supporting the importance of the increasing lung burden of silica in the occurrence of cancer. Overall, the authors concluded that the results support the carcinogenicity conclusion presented by IARC (1997).

To investigate the link between crystalline silica, silicosis and lung cancer, epidemiological data published between 1966 and 2001 were gathered. Over 50 studies were selected and pooled according to type of study and the parameter being linked to lung cancer (i.e. silica exposure, presence of silicosis in subjects). The quality of study, adjustment for confounding factors, co-exposure to other carcinogens and availability of a more recent analysis of a same cohort were taken into consideration in the final selection of the studies. Analysis of the relationship between exposure to silica and lung cancer included 17 cohort and 13 case-control studies. For the analysis of lung cancer versus silicosis, 11 cohort and 5 case-control studies were selected. The third analysis included 6 cohort and 2 case-control studies to evaluate the risk of lung cancer in non-silicotics. A random effect model was used to conduct each meta-analysis. Pooled cancer risk ratios (RRs) were 1.32 (CI 1.23-1.41) for crystalline silica exposure, 2.37 (CI 1.98-2.84) for individuals exposed to silica with confirmed silicosis (Silicotics) and 0.96 (CI 0.81-1.15) for individuals with no evidence of silicosis (non-silicotics) with confirmed exposure to silica, supporting the general observation that silicosis has a stronger temporal relationship with crystalline silica exposure and furthermore support the view that a human silicotic response could be a preliminary stage in the development of cancer.

A more recent meta-analysis included 28 cohort, 15 case-control and two proportionate mortality ratio (PMR) [See Appendix 1] studies from a variety of occupational settings conducted between 1996 and 2005. Risk ratios (RRs) were calculated based on type of study and silicosis status using fixed and random effect models (results presented here are from the random model). RRs for all cohort studies was 1.34 (CI 1.25-1.45), and were 1.69 (CI 1.32-2.16) for silicotics, 1.25 (CI 1.18-1.33) for those with undefined silicosis status and 1.19 (CI 0.87-1.57) for non-silicotics. In the case-control studies, the general RR was 1.41 (CI1.18-1.67), and the same sub-groups as mentioned above resulted in RRs of 3.27 (CI 1.32-8.2), 1.41 (CI1.18-1.70) and 0.97 (CI 0.68-1.38), respectively. The proportionate mortality ratio for the last two studies was 1.24 (CI 1.05-1.47). The authors noted that the association between lung cancer and exposure to crystalline silica was more consistent for silicotics, i.e., those diagnosed with silicosis and RR values split into type of occupational settings in which participants worked.

Based upon the above three meta-analysis studies and the epidemiology studies discussed in IARC (1997), the following can be concluded. Lung cancer rates are higher in workers confirmed to have silicosis versus similarly exposed workers that do not have silicosis. Cancer risk is often more significant in workers exposed to crystalline silica over a 20 year period or to higher cumulative exposure levels; however a consistent finding is that the onset of silicosis, requires a smaller lag period than that for the appearance of tumours. Similarly, cancer risk is often more significantly associated at higher quintiles of exposure compared to the lower quintiles.

There have been reports of tumours outside of the lungs in persons with high silica exposure; however, these reports are sparse and the data inconsistent and have not been unequivocally linked to exposure to either one of the crystalline forms (quartz or cristobalite). Some of the reported locations are: oesophagus, stomach, liver, skin and bone. Sufficient epidemiological or toxicological data do not currently exist for quantitative assessment of the exposure-response relationship on these other tissues or organs.

Genotoxicity

Potential genotoxicity has been assessed in multiple *in vitro* and *in vivo* assays. Table 1 below gives a brief summary of the positive results observed in each type of assay.

Table 1. Summary of positive results over total number of results for each assay and each category (all studies conducted with crystalline silica: quartz, except where indicated).

Assay	Animal data		Human data		Positives/Total	
	In vitro	In vivo	In vitro	In vivo[d]	In vitro	In vivo
Rec Assay	0/1				0/1	
DNA strand break	1/1	2/2	5/5[b]	1/1	6/6	3/3
Sister chromatid exchange	0/1		0/1[c]	1/1	0/2	1/1
Micronucleus	2/3	0/1	2/2[b]	1/1	4/5	1/2
Chromosome aberration	0/1			1/1	0/1	1/1
Aneuploidy/polyploidy	0/3				0/3	
Cell transformation	4/4				4/4	
Hprt mutation	1/2	2/2[a]	1/1[b]		2/3	2/2
Oxidative DNA damage		4/5	2/2		2/2	4/5
DNA binding		1/1				1/1
p53 activation		0/1				0/1

a. one assay conducted with crystalline silica: cristobalite
b. one assay conducted with "ultrafine crystalline silicon dioxide".
c. crystalline silica: tridymite
d. crystalline silica dust (subtypes not provided).

All the *in vivo* human genotoxicity studies are based on three independent studies that used blood samples from workers from diverse occupational settings with confirmed exposures to crystalline silica dust; however, quantification of exposure was not provided. After stratification by smoking status, sister chromatid exchange remained statistically significant in both smokers and non-smokers although the frequency was higher in smokers. For the chromosome aberration assay conducted as part of the same study (blood samples from workers in the stone crusher industry), the increased frequency was no longer significant after stratification. In the DNA damage study of foundry and pottery workers and the micronucleus assay of workers involved in sandblasting and related jobs, results were positive when compared to controls. However, in both studies, smoking status influenced the results, contributing to the increased DNA damage observed since results were greater in smokers versus non-smokers, and the frequency of micronuclei in nasal epithelial cells was higher in smokers ($p=0.002$) but when using peripheral blood lymphocytes did not differ statistically between smokers and non-smokers who were similarly exposed to silica dust,

The role of *in situ* generation of reactive oxygen species (ROS) and reactive nitrogen species (RNS) has been well established in the following types of DNA damage: small scale insertions, DNA base pair deletion, base modification, chromosomal change/loss, microsatellite instability, DNA strand break, 8-hydroxydeoxyguanosine (8-OHdG) mutation and point mutations. ROS and RNS generation is postulated to be (a part of) the DNA damage mechanism for crystalline silica. Studies are described below to support this hypothesis.

DNA was exposed *in vitro* to various crystalline silica dusts, to H_2O_2, or to both. Results show that DNA damage was limited when dust or H_2O_2 were administered alone but increased with the co-exposure. When the reactive oxygen scavenger, dimethylsulfoxide, was added to the test system, DNA strand break was inhibited, data supporting the viewpoint that it is the presence of radicals generated in response to quartz and cristobalite that causes the DNA damage and not quartz or cristobalite themselves.

Hprt mutation assays in rat alveolar epithelial cells, both *in vitro* and *in vivo,* were positive in response to quartz. The positive results *in vivo* were seen only in the presence of significant inflammatory responses in the treated animals. Also, in a parallel *in vitro* experiment, rat alveolar epithelial cells were incubated with the bronchoalveolar lavage fluid from the rats exposed to quartz. Both macrophage and neutrophil enriched lavage cells induced mutation in the exposed alveolar epithelial cells. Addition of catalase (an enzyme which inactivates H_2O_2) before incubation inhibited the increase in *hprt* mutation.

Rats were exposed to either crystalline or amorphous silica in a manner to induce the same level of inflammation in the lungs. The inflammatory response was assessed by measuring the proportion of neutrophils in the bronchiolar lavage fluid. The actual concentrations were 3 and 50 mg/m^3 for crystalline and amorphous silica respectively. The animals were exposed for 13 weeks. *Hprt* mutation frequency was measured in the alveolar epithelial cells at the end of the exposure period. Mutation frequency was greatly increased only in the crystalline silica treated rats; no treatment related increase was found in the rats treated with the amorphous form.

In an 8-OHdG assay conducted to monitor DNA damage by reactive oxygen species, female rats were exposed to 0, 0.3, 1.5 and 7.5 mg/animal of quartz via intratracheal instillation. Effects were observed 90 days post-exposure. A clear dose-response relationship was identified between quartz exposure and various inflammation markers (differential cell count, protein, lung surfactant lipids and tumour necrosis factor alpha). Inflammation was present starting at the lowest dose. However, 8-OHdG showed a statistically significant increase starting at 1.5 mg/animal only. Similarly, in another study, 8-OHdG and DNA strand breaks were observed at concentrations of or above 10 ug/m^3 in rat lung epithelial cells.

In the aim of investigating the role of ROS in lung carcinogenesis, rat lung epithelial cells were incubated with polymorphonuclear (PMN) leukocytes (involved in the inflammatory process and responsible for the release of certain ROS) or hydrogen peroxide. Statistically significant increases in 8-OHdG were observed in the presence of PMN or hydrogen peroxide in a dose-response manner.

In a series of experiments which used *in vitro* stimulation of macrophages with crystalline silica and *in vivo* intranasal instillation of crystalline silica in mice, it was demonstrated that that the chronic fibrosis seen in a murine model of silicosis *in vivo* is dependent on the presence of adaptor molecule ASC and Nalp3 inflammazome. These data support a potential mode of action whereby silica triggers cellular responses that in turn activate alveolar macrophages, resulting in an inflammatory response and silicosis. In mice deficient in Nalp3 inflammazome, the development of inflammation and collagen deposition was significantly reduced compared with normal mice 3 months after the initial intranasal instillation of silica.

Analysis of Lung Tumour Data

The weight of evidence for both rats and humans indicates that fibrotic and silicotic lesions in the lung result from inhalation exposure to crystalline silica and that lung cancer is secondary to those lesions in the lung. Although the mechanism of induction for the lung tumours has not been fully elucidated, there is sufficient supportive mode of action evidence from the data presented to demonstrate that a threshold approach to risk assessment is appropriate based on an understanding of the key events in the pathogenesis of crystalline silica induced lung tumours. The body of evidence include the following:

- In experimental studies, all rats that developed tumours also showed fibrosis.
- Adenocarcinomas, the most common type of tumour identified in rats, are commonly associated with fibrosis and deeply scarred lung tissue.
- Experimental rat studies showed a clear progression of the effects from initially mild inflammation, followed by fibrosis over-time, leading eventually to lung tumours.
- Tumours are not present in all treated species dosed in the same way.
- The tumours, both in rats and humans, are concentrated in the lungs only, although other organs are indirectly exposed.
- In human studies, cancer risk is often more significant in workers exposed over a 20 year period or to higher cumulative exposure levels; however a consistent finding is that the onset of silicosis, requires a smaller lag period than that for the appearance of tumours.
- Similarly, cancer risk is often more significantly associated at higher quintiles of exposure compared to the lower quintiles
- Lung cancer rates are higher in workers confirmed to have silicosis versus similarly exposed workers that do not have silicosis.
- For genotoxicity, in vitro results were mostly mixed and in vivo results were mostly positive. However, the vast majority of the positive genotoxicity assay results can be explained by the generation of reactive oxygen species, as demonstrated experimentally, where ROS scavenging prevents the genotoxicity.
- *In vivo*, macrophage deficient mice (macrophages produce ROS in response to crystalline silica) do not develop silicosis nor do they develop tumours and the Nalp3 inflammazome, a key player in the

macrophage initiated inflammatory response, is required for the development of pulmonary fibrosis after inhalation of silica.

- Though inhalation exposure to crystalline silica in multiple occupational settings is clear, the increase in risk, based on the several recent meta-analyses of the multiple human epidemiological studies, remains low.

It is worth noting that where aggressive engineering controls have been made to reduce silica dust levels in the workplace (Sweden), silicosis has been eliminated. By corollary, existing exposures outside of the workplace in such areas do not pose a risk for silicosis to the general population.

The respirable forms of quartz and cristobalite possess properties indicating a hazard for human health (repeated dose toxicity, carcinogenicity and genotoxicity). The mode of action in the lungs involves irritation, inflammation and reactive species formation, leading to silicosis, and eventually to tumour formation.

Exposure

Uses

Consistent with oxygen and silicon being the two most abundant elements in the Earth's crust, silicon-oxide minerals, including quartz are ubiquitous in the natural environment. In particular, as a component of sand, quartz may find use in a diverse array of applications. Several high volume uses include, but are not limited to, the use of sand as a filling material for the construction of roads and in general building activities, the use of sand and gravel aggregates as abrasives on roads in winter and the use of fly-ash, which may contain 4-14% quartz and 0.5-1% cristobalite, as a cement additive. These abrasives when used on winter roads are usually mixed with road salts and may be sand only, stone dust, sand and gravel aggregates, or pre-treated sand. They are used mainly by rural municipalities or in areas where cold temperatures diminish the efficiency of salts for de-icing. Quantities of abrasives used in Canada were 5.73×10^9 kg, 4.59×10^9 kg, and 4.93×10^9 kg for 2007, 2008 and 2009, respectively.

Industrial sand, high purity silica sand products with closely controlled sizing are expected to contain quartz and cristobalite, include lump silica (2-3mm up to 15 cm or more), silica sand (75µm to 2-3mm) and silica flour (less than 75µm). Lump silica may be used in the production of silicon alloys, silica bricks, and the linings of certain types of pulverizers (eg. ball mills and tube mills).

Silica sand may be used in the manufacture of glass and glass fibres, silicate chemicals and silicon carbide, the hydraulic fracturing of wells, foundry moulding, and for sandblasting. Silica flour may find use in the ceramics and cement industries, as a filler and extender in rubber and coatings, and as an abrasive in soaps.

Natural clays, such as bentonite and fuller's earth, are used in cat litters for their high water absorbance capacities. Quartz is a natural component of these clays, and consequently, it may be present in cat litter products. High purity α-quartz is a piezoelectric material, which means that application of a voltage induces a distortion in the crystal shape and vice versa. This ability to interconvert electrical and mechanical energy has led to the use of quartz crystals in electronic devices requiring precise timing control, for example telephones, radios, watches and computers.

According to a survey conducted in Canada, quartz and cristobalite are also used in abrasives, adsorbents, filter products (diatomaceous earth), grout and cement. These substances reportedly also find use as fillers, which add bulk and improve wear resistance, in paints and coatings, adhesives, sealants, polymer films, caulking, epoxy resins and silicones. Also, quartz is listed as an ingredient in 60 cosmetic products in Canada. The types of products include anti-wrinkle preparation, eye and face makeup, lipstick, hair dyes, shampoos and grooming products, as well as skin cleansers, moisturizers and tanning preparations.

Natural Sources

In Canada, quartz naturally occurs in many types of rock formations. Those with high silicon dioxide content (95% SiO_2 or more) include vein and massive intrusion bodies, quartz pebbles, silica sand, sandstone and quartzite. Sandstone is a sedimentary rock mostly composed of quartz grains cemented by a bonding material such as clay, calcite or iron oxide. Quartzite is a hard, compact, metamorphosed sandstone made of grains of quartz firmly bonded with a siliceous cement. Mineral aggregates (e.g., sand and gravel) have variable silicon dioxide content. Quartz is also found as crystals, aggregates or discrete particles in certain igneous rocks (e.g., granites and pegmatites), soils, sediments, air and surface water. This omnipresence is consistent with the fact

that silicon is the second most abundant chemical element on Earth.

Cristobalite is naturally produced in the ashes of volcanic eruptions, and by combustion metamorphism which is a local phenomenon of spontaneous combustion of naturally occurring substances such as bituminous rocks, coal or oil. It may be found in cavities in volcanic rocks and in thermally metamorphosed sandstones and may also be a transient stage in the diagenesis of diatomaceous shale with the result that soils made of these geologic formations may be rich in cristobalite. Unlike quartz, the natural occurrence of cristobalite is limited to specific geographic regions and mineral types.

Anthropogenic Sources

Natural quartz is isolated from ore via beneficiation, which involves milling or grinding the material into particles that are separated into desired mineral and waste. The materials obtained are either used directly or further purified. In Canada, in 2006, 2.146×10^{9} kg of pure quartz were mined, and 2.385×10^{11} kg of sand and gravel aggregates were produced. The proportion of quartz in silica sand deposits and gravel aggregates will vary from one site to another.

Cristobalite can form from silica melts during the preparation of silica glass; quartz is not obtained from melts but is manufactured at elevated temperature and pressure via a hydrothermal process. Cristobalite also forms during the calcination[2] of diatomaceous earth.

Human Exposure Estimate

Ambient air

The exposure assessment is focussed on respirable quartz and cristobalite, which in ambient air comprises a component of total particulate matter (PM). In Canada, data on the concentrations of silicon in PM was available and used as a surrogate for quartz and cristobalite. This approach is conservative because the measured silicon includes all silicon-containing substances and therefore represents the upper limit for quartz and cristobalite in ambient air.

The National Air Pollution Surveillance (NAPS) Program measured concentrations in $\mu g/m^3$ of silicon in PM with aerodynamic radii less than 2.5 µm ($PM_{2.5}$ (dichot)), and from 2.5 to 10 µm (PM_{10} (dichot)) (the total particulate matter with aerodynamic radii less than 10 µm (PM_{10}) is obtained by adding these values) in Canada. In 2009, as part of the NAPS Program, silicon concentrations were determined on over 1600 samples of $PM_{2.5}$(dichot) and over 1500 samples of PM_{10}(dichot) at 24 urban locations across Canada. An estimate of exposure to quartz and cristobalite can be obtained by assuming that all the silicon in the PM is represented stoichiometrically as SiO_2, and multiplying the reported concentration of silicon by 2.14 to obtain a value for silica.

The intake of respirable quartz and cristobalite by the general population of Canada is estimated using a range covering the lowest 50^{th} percentile SiO_2 concentration in PM_{10}, measured in Pt. Petre, ON, (0.12 $\mu g/m^3$) to the highest 50^{th} percentile concentration in PM_{10} measured in Calgary, AB (2.1 $\mu g/m^3$). The 50^{th} percentile SiO_2 concentrations ranged from 0.1 to 2.1 $\mu g/m^3$ across the survey sites; the top of this range is quite close to the average of the maximum values for the 24 sites (3.7 $\mu g/m^3$). The outdoor data were used to represent the indoor levels, because information on indoor silicon concentrations was not available, and the range of PM_{10} measured indoors is generally lower than the outdoor range. Thus, this approach conservatively overestimates indoor exposure in homes.

The highest exposure group based on these calculations is children ages 0.5 to 4 years with an estimated daily intake ranging from 0.07 to 5.26 µg/kg-bw per day; the estimated daily intake decreases with age due to changes in the ratio of inhalation rates to body weights; the daily intake of adults, 20-59 years old, is estimated to range from 0.03 to 2.00 µg/kg-bw per day.

Consumer Products

Exposure to respirable quartz from the use of cosmetic products, which contained quartz as an ingredient, was considered low because they are not formulated for spray application, the loose powders were reported to contain less than 0.1% quartz, and in these products the substance is not expected to be associated with other components of the formulation and not available in a free form.

For consumer Do It Yourself (DIY) activities around the home, the highest mean breathing zone concentration

[2] Calcinations: Heat treating a substance, but without fusion, to bring about change in its physical or chemical constitution.

of particles from sanding dry wall (median cut-point of 10μm) of 6.31 mg/m^3, was used to derive an upper-bound exposure estimate ranging from 2 to10 μg/kg-bw per event.

Quartz is used to formulate a large number of paints and coatings. To estimate potential inhalation exposure to quartz from these products, the spray painting of wall paints with an airless spray gun was considered appropriate as a conservative scenario. Exposure to respirable paint particles was estimated using data from controlled a laboratory study in which walls of poorly ventilated test rooms were painted by professional painters using an airless sprayer to apply interior latex paint. The maximum concentration of 13% quartz in paint in Canada was used to estimate exposure. The upper-bound estimate of exposure to quartz, based on the maximum concentration of 13% quartz in paint in the Canadian market and the maximum concentration of respirable paint particles measured in these controlled studies when recommended personal protective equipment is used, is 0.954 μg/kg-bw per event.

Inhalation of ambient air containing quartz and cristobalite is the dominant pathway of chronic exposure (excluding that from DIY activities) for the general population. Because SiO_2 makes up only approximately 5% of PM_{10}, silicon concentrations (expressed as SiO_2) measured in the Canadian NAPS survey of 24 urban locations were considered most relevant to the estimation of exposure by the general population. Quartz and cristobalite comprise only a portion of the total SiO_2 in PM_{10}, therefore, the use of the total silicon concentration to represent the upper bound crystalline silica concentrations results in an overestimation of exposure.

Appendix 1: Definitions of Epidemiological Terms in the ITAP

SMR (Standardized Mortality Ratio): The ratio (x 100) of observed to expected deaths in a study population. Expected deaths are calculated by applying a set of standard age-specific mortality rates to the age distribution of the study population. Standardized ratios are only useful for comparisons. They have no intrinsic meaning.

OR (Odds Ratio): In epidemiological case-control studies, a relative measure of disease occurrence. The odds in favour of a particular disease occurring in an exposed group are divided by the odds in favour of its occurring in an unexposed group. If the condition being studied is rare, the odds ratio is a close approximation to the relative risk.

RR (Risk Ratio): The probability of the occurrence of a disease in a group that has been exposed to some environmental, medicinal, microbial, or toxic influence, relative to its probability in a randomly selected population.

PMR (Proportionate Mortality Ratio): Proportionate mortality is the proportion of deaths in a specified population over a period of time attributable to different causes. Each cause is expressed as a percentage of all deaths, and the sum of the causes must add to 100%. These proportions are not mortality rates, since the denominator is all deaths, not the population in which the deaths occurred. Thus, proportionate mortality ratio is a measure of the frequency of occurrence of the proportionate mortality in a defined population during a specified interval of time.

DIETHYLENE GLYCOL MONOBUTYL ETHER

This dossier on diethylene glycol monobutyl ether (DGBE) presents the most critical studies pertinent to the risk assessment of DGBE in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – DGBE is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

DGBE is readily biodegradable. It is not expected to bioaccumulate. DGBE has a low tendency to bind to soil or sediment.. DGBE is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-(2-butoxyethoxy)ethanol

CAS RN: 112-34-5

Molecular formula: $C_8H_{18}O_3$

Molecular weight: 162.23 g/mol

Synonyms: Diethylene glycol monobutyl ether; 2-(2-butoxyethoxy)ethanol; diethylene glycol butyl ether; ethanol, 2-(2-butoxy)-; butyldiglycol ether; butyl dioxitol

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of DGBE

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid with a faint, butyl odour.	2	ECHA
Melting Point	<-70°C @ 101.3 kPa	2	ECHA
Boiling Point	231°C @ 101.3 kPa	2	ECHA
Density	955 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	2.9 Pa @ 25°C	2	ECHA
Partition Coefficient (log Kow)	1.0 @ 20°C	1	ECHA
Water Solubility	955 g/L @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Dissociation Constant (pKa)	14.8 @ 20°C	2	ECHA
Viscosity	6 mPa.s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (**Table 2**). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for DGBE.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

DGBE is readily biodegradable. It is not expected to bioaccumulate. DGBE has a low tendency to bind to soil or sediment.

B. Biodegradation

DGBE is readily biodegradable. In an OECD TG 301C test, there was approximately 85% degradation after 28 days as measured by O_2 consumption (ECHA) [Kl. score = 1]. In an OECD TG 301 B test, degradation was 64%, 74.3% and 87.1% after 13, 16 and 22 days, respectively (ECHA) [Kl. score = 2]. In a Zahn-Wellens (OECD TG 302 B) test, degradation was 99% after 8 days as measured by DOC removal (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for DGBE. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 4.387 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 10 L/kg.

Based upon these K_{oc} values, if released to soil, DGBE is expected to have low potential for adsorption and a high potential for mobility. If released to water, based on its K_{oc} and high water solubility values, DGBE is likely to remain in water and not adsorb to sediment.

D. Bioaccumulation

No bioconcentration studies have been conducted on DGBE. DGBE is not expected to bioaccumulate based on the experimental log K_{ow} of 1.0 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

DGBE is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on DGBE.

Table 3 Acute Aquatic Toxicity Studies on DGBE

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Lepomis machrochirus	96-hour LC_{50}	1,300	2	ECHA
Pimelphales promelas	96-hour LC_{50}	2,500	2	ECHA
Daphnia magna	48-hour EC_{50}	>100	1	ECHA
Daphnia magna	48-hour EC_{50}	2,850	2	ECHA
Daphnia magna	24-hour EC_{50}	3,200	2	ECHA
Daphnia magna	48-hour EC_{50}	4,950	2	ECHA
Daphnia magna	48-hour EC_{50}	>1,000	2	ECHA
Scenedesmus subspicatus	96-hour EC_{50}	>100 (growth rate) >100 (biomass)	1	ECHA
Scenedesmus subspicatus	72-hour EC_{50}	1,101 (growth rate)	2	ECHA

Chronic Studies

The 96-hour NOEC from an algal study using *Scenedesmus subspicatus* were >100 mg/L for growth rate and biomass (ECHA). [Kl. score = 1]

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

DGBE is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 1.0, DGBE does not meet the screening criteria for bioaccumulation.

The 96-hour NOEC from an algal study on DGBE is >0.1 mg/L. The acute EC_{50} values for DGBE are >1 mg/L in fish, invertebrates and algae. Thus, DGBE does not meet the screening criteria for toxicity.

The overall conclusion is that DGBE is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for DGBE.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Diethylene Glycol Monobutyl Ether	112-34-5	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

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USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DGBE	diethylene glycol monobutyl ether
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry

kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litre per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligram per litre
mm	millimetre
mPa s	millipascal second
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TG	Test Guideline

DIAMMONIUM PEROXODISULPHATE

This dossier on diammonium peroxodisulphate presents the most critical studies pertinent to the risk assessment of diammonium peroxodisulphate in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Diammonium peroxodisulphate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Diammonium peroxodisulphate is an inorganic compound. It is highly soluble in water, dissociating into respective cations and anions. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. Diammonium peroxodisulphate is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Diammonium peroxodisulphate

CAS RN: 7727-54-0

Molecular formula: $H_8N_2O_8S_2$

Molecular weight: 228.21 g/mol

Synonyms: Diammonium peroxydisulfate; Diammonium peroxydisulphate; Diammonium persulfate; Peroxydisulfuric acid (((HO)S(O)2)2O2), ammonium salt (1:2); Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt; Peroxydisulfuric acid, diammonium salt; ammonium persulphate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Diammonium Peroxodisulphate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, odourless, crystalline solid	1	ECHA
Melting Point	ND. Decomposes at ca. 120°C at 100.66 kPa	1	ECHA
Boiling Point	ND. Decomposes at ca. 393 K (= 120°C) at 100.79 kPa	1	ECHA

Property	Value	Klimisch score	Reference
Density	1260 kg/m³ at 20°C	1	ECHA
Vapour Pressure	0 Pa @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable as substance is inorganic salt	-	ECHA
Water Solubility	850 g/L @ 25°C	2	ECHA
Viscosity	ND. Substance is a solid at room temperature	-	ECHA
Dissociation constant (pKa)	Diammonium persulfate dissociates completely to ammonium cation and persulfate anion when it is dissolved in water.	-	ECHA

ND – not determined

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for diammonium peroxodisulphate.

NICNAS has assessed diammonium peroxodisulphate in an IMAP Tier 1 environmental assessment and it was concluded that it poses no unreasonable risk to the environment[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7727-54-0

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Diammonium peroxodisulphate dissociates in aqueous media to the ammonium cation and persulfate anion. Biodegradation is not applicable to inorganic compounds. Diammonium peroxodisulphate is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Diammonium peroxodisulphate is not expected to adsorb to soil or sediment because of its dissociation properties and high water solubility.

B. Partitioning

Persulfates dissociate in water to the corresponding cation and persulfate anion. Hydrolysis is temperature and pH dependent. The persulfate anion, independent from the cation, undergoes decomposition in normal water or acid conditions, readily oxidizing water to oxygen, producing acid conditions. All degradation products are ubiquitous to the environment (ECHA).

Diammonium peroxodisulphate was shown to be hydrolytically stable at 10 °C and pH 4, 7 and 9, a minor hydrolysis was observed at 25 °C, whereas, a very strong hydrolysis at 60 °C was observed within 4 days. The DT50 at pH 4 and 60 °C was determined to be 27.2 h, at pH 7 and 9 and 60 °C the DT50 was determined to be 36.5 h. The DT50 at environmentally relevant temperature (12 °C) and pH 7 was extrapolated to be 1698.18 h (70.76 d). (ECHA) [Kl. Score = 1].

C. Biodegradation

Biodegradation is not applicable to inorganic compounds.

D. Environmental Distribution

No experimental data are available for diammonium peroxodisulphate. Persulfates are soluble in water and their vapour pressures are negligible. Thus, persulfates released into the environment are distributed into the water compartment in ionic form of the cation and persulfate ion. Persulfates are not expected to sorb to soil due to their dissociation properties, instability (hydrolysis) and high water solubility. They behave as free ions and decompose into sulfate and bisulfate ions. All decomposition products are ubiquitous in the environment (ECHA).

E. Bioaccumulation

There are no bioaccumulation studies on diammonium peroxodisulphate. Substances of the Persulfate Category are inorganic salts sharing the same anionic persulfate moiety. Persulfates are very soluble in water and are not expected to bioaccumulate in soil or aqueous solutions. They will decompose into organic sulfate or bisulfate (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Diammonium peroxodisulphate is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on diammonium peroxodisulphate.

Table 3 Acute Aquatic Toxicity Studies on Diammonium Peroxodisulphate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	76.3 mg/L	1	ECHA
Daphnia magna	48-hour EC_{50}	120 mg/L	1	ECHA
Phaeodactylum tricornutum	72-hour EC_{50}	320 mg/L	1	ECHA

Chronic Studies

Long-term toxicity testing to fish was considered scientifically unjustified, due to the results obtained in the short-term toxicity to fish studies, the substance physical-chemical properties and hydrolysis behaviour (ECHA).

An OECD Guideline 211 (Daphnia magna Reproduction Test) was performed and yielded a 21-day NOEC of 20.8 mg/L based on reproduction (ECHA) [Kl Score = 1].

C. Terrestrial Toxicity

No terrestrial toxicity studies are available.

Persulfates are not expected to be distributed into the terrestrial compartment and consequently not to cause toxicity to terrestrial organisms and plants (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Diammonium peroxodisulphate is an organic salt that dissociates to respective cations and anions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Diammonium peroxodisulphate is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Thus, the substance does not meet the screening criteria for bioaccumulation.

Chronic aquatic toxicity data is > 0.1 mg/L and acute aquatic toxicity data is >1 mg/L. Thus, diammonium peroxodisulphate does not meet the screening criteria for toxicity.

The overall conclusion is that diammonium peroxodisulphate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for diammonium peroxodisulphate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Diammonium peroxodisulphate	7727-54-0	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
K	Kelvin
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SGG	Synthetic Greenhouse Gases

DIETHANOLAMINE

This dossier on diethanolamine (DEA) presents the most critical studies pertinent to the risk assessment of diethanolamine in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion –Diethanolamine is classified as a **tier 1** chemical and requires a hazard assessment only. A review of aquatic toxicity data indicates that overall (18 of 26 acute and chronic tests reviewed in ECHA) would classify the substance as tier 1. Moreover, the substance has been determined to biodegrade in the environment very quickly suggesting that chronic toxicity would be less relevant than acute toxicity (where 15 of 17 tests support the tier 1 classification).

1 BACKGROUND

Diethanolamine is readily biodegradable. It is not expected to bioaccumulate; and it has low potential to adsorb to soil. Diethanolamine exhibits moderate acute toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2,2'-iminodiethanol

CAS RN: 111-42-2

Molecular formula: $C_4H_{11}NO_2$

Molecular weight: 105.14 gm/mol

Synonyms: Diethanolamine; 2,2'-iminodiethanol; 2,2'-dihydroxydiethylamine; 2-[(2-hydroxyethyl)amino]ethanol; bis(2-hydroxyethyl)amine; DEA; di(2-hydroxyethyl)amine; ethanol, 2,2'-iminobis-(9Cl); ethanol, 2,2'iminodi-(8Cl)

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Diethanolamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid Crystals (prisms) or syrupy liquid	2	ECHA
Melting Point	27°C @ 101.3 kPa	1	ECHA
Boiling Point	268.9°C (decomposition occurs >200°C) @ 101.3 kPa	1	ECHA

Property	Value	Klimisch score	Reference
Density	1100 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	0 Pa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	-2.46 @ 25°C	2	ECHA
Water Solubility	1000 g/L @ 20 °C (miscible)	2	ECHA
Dissociation Constant (pKa)	8.99 @ 20°C	2	ECHA
Viscosity	390.9 mPa.s @ 30°C; 102.7 mPa.s @ 50°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for diethanolamine.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Diethanolamine is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to soil.

B. Partitioning

Diethanolamine is highly soluble in water. Based on its Henry's Law Constant is not expected to evaporate into the atmosphere from the water surface. However, the substance will be rapidly degraded by photochemical processes (half-life = 4.2 h).

C. Biodegradation

Diethanolamine is readily biodegradable. In an OECD 301F test, there was 50% degradation after 7 days, 80% after 14 days, and 93% after 28 days (OECD, 2007; ECHA) [Kl. score = 1]. In a "Ready"

Biodegradability – Dissolved Organic Carbon (DOC) Die-Away test, there was 86% degradation after 7 days and 96% degradation after 10 days (ECHA) [Kl. score = 2]. In modified OECD 301E screening tests using river or pond water, there was 93% and 97% degradation (measured as DOC removal) after 28 days (OECD, 2007; ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for diethanolamine. The K_{oc} for diethanolamine (as the charged molecule) was calculated to be 10 at pH values between 5 and 8 (Franco and Trapp, 2008; Franco et al., 2009; ECHA). [Kl. score = 2]

If released to water, based on its low K_{oc} and high water solubility values, diethanolamine is likely to remain in water and not adsorb to sediment. It is also not expected to adsorb to soil, and, has the potential to be highly mobile. However, the mobility of the substance is dependent on the cation exchange capacity of the soil (Government of Alberta, 2010)

E. . Bioaccumulation

There are no bioaccumulation studies on diethanolamine. The BCF was estimated to be 2.3 based on calculations from OASIS Catalogic v.5.11.15 [BCF base-line model v.0208] (Dimitrov et al., 2005; ECHA). Based on the log K_{ow} (-2.46) and the calculated BCF, bioaccumulation is not to be expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Diethanolamine exhibits moderate acute toxicity to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on diethanolamine.

Table 3 Acute Aquatic Toxicity Studies on Diethanolamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	460	2	ECHA
Pimephales promelas	96-hour LC_{50}	1,460*	2	Mayes et al. (1983)
Pimephales promelas	96-hour LC_{50}	1,664	2	ECHA
Lepomis macrochirus	48-hour LC_{50}	1,850	2	Turnbull et al. (1954)
Carassius auratus	24-hour LC_{50}	>5,000 (neutralised) 800 (non-neutralised)	2	Bridié et al. (1979)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Ceriodaphnia dubia	48-hour EC_{50}	30.1 (24°C) 89.9 (20°C)	2	Cowgill et al. (1985)
Daphnia magna	48-hour EC_{50}	55	2	LeBlanc (1980)
Daphnia magna	48-hour EC_{50}	171	2	Zurita et al. (2005)
Pseudokirchneriella subcapitata	72-hour EC_{50} (growth rate)	9.5 (Test 1) 19 (Test 2)	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	14.9 (growth rate) 6.2 (biomass)	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	107.3 (growth rate) 74.5 (biomass)	2	ECHA
Chorella vulgaris	72-hour EC_{50}	778 (growth rate)	2	ECHA

*Geometric mean of 96-hour LC_{50} values of fry, juvenile and subadult fish. Not neutralised.

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies on diethanolamine.

Table 4 Chronic Aquatic Toxicity Studies on Diethanolamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	EC_{10} NOEC	1.05 0.76	1	ECHA
Pseudokirchneriella subcapitata	EC_{10} (growth rate)	1.4 (Test 1) 1.1 (Test 2)	2	ECHA
Desmodesmus subspicatus	EC_{10} (neutralised)	2.4 (growth rate) 2.0 (biomass)	2	ECHA
Desmodesmus subspicatus	EC_{10} (non-neutralised)	85.7 (growth rate) 41.3 (biomass)	2	ECHA
Pseudokirchneriella subcapitata	7-day NOEC	10	2	ECHA

C. Terrestrial Toxicity

In an earthworm (*Eisenia Andrei, Eisenia fetida*, or *Lumbricus terrestris*) study, the 35-day LC_{50} was 4,141 mg/kg soil dry weight (mortality); the 63-day EC_{50} was 776 mg/kg soil dry weight (reproduction); and the 63-day EC_{25} was 171 mg/kg soil dry weight (reproduction) (ECHA). [Kl. score = 2]

In a springtails (*Folsomia candida*) study, the 28-day LC_{50} was 8,301 mg/kg soil dry weight (mortality); the 28-day EC_{50} was 4,205 mg/kg soil dry weight (reproduction); and the 28-day EC_{25} was 2,102 mg/kg soil dry weight (reproduction) (ECHA). [Kl. score = 2]

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Diethanolamine is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The estimated BCF value for diethanolamine calculated from a QSAR model is 2.3; thus, it does not meet the criteria for bioaccumulation.

The EC_{10} or NOEC values from the chronic aquatic toxicity studies on diethanolamine are >0.1 mg/L. Thus, diethanolamine does not meet the screening criteria for toxicity. In a mouse dermal carcinogenicity study, there was an increased incidence of liver tumours in males and females and kidney tumours in males. However, both ECHA and NICNAS have concluded that "[t]he data on the mode of action are insufficient to conclude that diethanolamine-induced tumours in mice are relevant for humans and, therefore, based on the available information, diethanolamine is not classified for carcinogenicity." Thus, diethanolamine does not meet the criteria for toxicity.

Therefore, diethanolamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for diethanolamine

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Diethanolamine	111-42-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

^{o}C	degrees Celsius
^{o}F	degrees Fahrenheit
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg/kg	milligram per kilogram
mg/L	milligram per litre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic

QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

DIETHYLENE GLYCOL

This dossier on diethylene glycol presents the most critical studies pertinent to the risk assessment of diethylene glycol in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Diethylene glycol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Diethylene glycol is derived as a co-product with ethylene glycol (MEG) and triethylene glycol. The industry generally operates to maximize MEG production. Ethylene glycol is by far the largest volume of the glycol products in a variety of applications. Availability of diethylene glycol will depend on demand for derivatives of the primary product, ethylene glycol, rather than on diethylene glycol market requirements.

Diethylene glycol is readily biodegradable and unlikely to bioaccumulate. Diethylene glycol has low potential to adsorb to soil and sediment. Diethylene glycol is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2,2'-oxydiethanol

CAS RN: 111-46-6

Molecular formula: C_4H10O_3 or $(CH_2CH_2OH)_2O$

Molecular weight: 106.12 g/mol

Synonyms: Diethylene glycol; 2,2'-oxydiethanol; diglycol; bis(2-hydroxyethyl) ether; 2-hydroxyethyl ether; 2,2'-oxybisethanol; 2-(2-hydroxyethoxy)ethanol; ethanol, 2,2'-oxybis-; 2-(2-hydroxyethoxy)ethan-1-ol; glycol ethyl ether; ethylene diglycol.

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Diethylene Glycol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	A colorless viscous liquid	2	ECHA
Melting point	-6.5°C @ 101.3 kPa	2	ECHA
Boiling point	244.9°C @ 101.3 kPa	2	ECHA
Density	1,118 kg/m^3 @ 20°C	2	ECHA
Vapor pressure	0.008 hPa @ 25°C	2	ECHA
Partition coefficient (log K_{ow})	-1.98 (calculated)	2	ECHA
Water solubility	1,000 g/L @ 20°C	2	ECHA
Viscosity	30 mPa s (dynamic) @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for diethylene glycol.

NICNAS has assessed diethylene glycol in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=111-46-6%2C+

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

The substance is readily biodegradable, is unlikely to bioaccumulate, nor is it likely to adsorb or desorb to soil or sediment to a great extent.

B. Biodegradation

Diethylene glycol is readily biodegradable. In an OECD 301B test, there was 70-80% and 90-100% degradation after 28 days, as determined by CO2 evolution and DOC removal respectively (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

In an OECD 301A test, there was 90-100% degradation after 28 days, although the 10-day window was missed (ECHA) [Kl. score = 1]. In a modified MITI I test (OECD 301C), there was up to 92% degradation after 28 days (ECHA) [Kl. score = 2].

C. Environmental Distribution

No experimental data are available for diethylene glycol. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} value from the molecular connectivity index (MCI) and log K_{oc} are 1 and -0.08 L/kg, respectively (ECHA) [Kl. Score = 2]. Based on these K_{oc} values, if released to soil, diethylene glycol is expected to not adsorb to soil and have a very high mobility. If released to water, based on the K_{oc} value and its water solubility, it is also not expected to adsorb to suspended solids and sediment.

D. Bioaccumulation

The calculated log Kow for diethylene glycol is -1.98 (Verschueren, 1983). Diethylene glycol has low potential to bioaccumulate. In a three-day bioaccumulation fish study with Leuciscus idus melanotus, the BCF was determined to be 100 (Freitag et al., 1985) [Kl. score = 2].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance is of low toxicity concern to aquatic organisms.

A. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on diethylene glycol.

Table 3: Acute Aquatic Toxicity Studies on Diethylene Glycol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-h LC_{50}	75,200	2	ECHA
Oncorhynchus mykiss	96-h LC_5	66,000	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	24-h EC_{50}	>10,000	2	ECHA
Daphnia magna	48-h EC_{50}	65,980	2	ECHA
Daphnia magna	48-h EC_{50}	62,630	2	ECHA

Chronic Studies

In ECHA, the aquatic toxicity of the 'ethylene glycol and higher glycols' (mono-, di-, tri-, tetra- and pentaethylene glycol) is evaluated in a read-across approach. Data on all three trophic levels (fish, daphnia, algae) are available to describe the aquatic toxicity of the glycol read-across members. Due to the fact, that not for each single substance data for all required endpoints are available, a weight of evidence approach is used, which includes additional information based on QSAR calculation with the EpiWin-Program ECOSAR v1.11. Measured data as well as estimated data demonstrate, that all glycols within the read-across are not harmful to aquatic organisms. No adverse effects on aquatic organisms occurred up to concentrations above 100 mg/L (ECHA).

No data for fish was available for diethylene glycol. However, chronic studies for fish are available for ethylene glycol (CAS-No.: 107-21-1). The 7-day NOEC for the fathead minnow (*Pimephales promelas*) was determined to be 15,380 mg/L based on the weight of the test organisms (ECHA) [Kl. Score = 2].

No data for invertebrates was available for diethylene glycol. However, three studies were conducted with Dapnids (*Ceriodaphnia dubia* or *Daphnia magna*) for ethylene glycol (CAS-No.: 107-21-1) or triethylene glycol (CAS No.: 112-27-6). The study with ethylene glycol was conducted according to EPA guideline 600/4-89/001 with *Ceriodaphnia dubia* as test species. The 7-day NOEC for reproduction was determined to be 8,590 mg/L ethylene glycol (nominal). Two studies measured the effect of triethylene glycol on the reproduction of *Daphnia magna*. One study was conducted according to the national standard ASTM (E 47.01, Draft No. 1, "Draft proposed standard practice for conducting renewal life cycle toxicity tests with Daphnia magna"). In this test the Daphnids were exposed to triethylene glycol for 21 days. Based on reproduction the reported NOEC is > 15,000 mg/L triethylene glycol (nominal). (ECHA) [Kl. Score = 2].

Data for algae was available for diethylene glycol. The 8-day TGK to algae *Scenedesmus quadricauda* was determined to be 2,700 mg/L for diethylene glycol (ECHA) [Kl. score = 2].

From the QSAR calculations it can be expected for diethylene glycol that algae are slightly more sensitive (ChV = 1,200 mg/L) than invertebrates (ChV = 1,891 mg/L) or fishes (ChV = 7,694 mg/L). (ECHA) [Kl. Score = 2].

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Diethylene glycol has been shown to be readily biodegradable; thus, it does not meet the screening criteria for persistence. The calculated log $K_{ow}$is -1.98, and the experimental BCF is 100. Thus, diethylene glycol does not meet the screening criteria for bioaccumulation.

The lowest chronic toxicity value for diethylene glycol is >0.1 mg/L. Thus, diethylene glycol does not meet the criteria for toxicity.

Therefore, diethylene glycol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for diethylene glycol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Diethylene glycol	111-46-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = Bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry

kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

DIMETHYLSILOXANE, ETHYLENE OXIDE BLOCK COPOLYMER (POLYSILOXANE)

This dossier on dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) presents the most critical studies pertinent to the risk assessment of this substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is classified as a **tier 1** chemical and requires a hazard assessment only.

1. BACKGROUND

Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) belongs to a group of polymeric organosilicon compounds that are commonly referred to as silicones with use as a lubricant, levelling aid, anti-fog and anti-static agent.

Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is not readily biodegradable, is not expected to bioaccumulate nor be substantially toxic to environmental receptors.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 3-(2-methoxyethoxy)propyl-methyl-bis(tri27306-methylsilyloxy)silane

CAS RN: 27306-78-1

Molecular formula: $(C_2H_4O)_nC_{11}H_{30}O_3Si_3$ [This substance is a polymer]

Molecular weight: polymer variable (UVCB)

Synonyms: dimethylsiloxane, ethylene oxide block copolymer; polyethylene glycol monomethyl ether mono[3-[methylbis(trimethylsiloxy)silyl]propyl] ether; Silwet L 77

3. PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Dimethylsiloxane, ethylene oxide block copolymer

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Pale yellow clear viscous liquid with polyether odour	-	MPM, 2021a
Melting Point	Not Available	-	MPM, 2021a
Boiling Point	> 205°C (pressure not provided)	-	MPM, 2021a
Density	1,007 kg/m^3 @ 25°C	-	MPM, 2021a
Vapour Pressure	< 133 Pa @ 20°C	-	MPM, 2021a

Property	Value	Klimisch score	Reference
Partition coefficient (log K_{ow})	> 3.29 @ pH 5	-	MPM, 2021a
Water Solubility	Miscible	-	MPM, 2021a
Viscosity	24 mPA s (dynamic) (temperature not provided)	-	MPM, 2021a

*Based on Material Safety Data Sheet (MSDS) for Silwet L 77, lowest molecular weight hydrophilic silicone containing 6 – 8 ethylene oxide (EO) units

Dimethylsiloxane, ethylene oxide block copolymer is a hydrophilic silicone. Hydrophilic silicones differ from conventional silicones by demonstrating a much greater compatibility with aqueous systems. They have slight to complete solubility in water. They are composed of dimethylsiloxane molecular backbones in which some of the methyl groups are replaced by polyalkylenoxy or pyrrolidone groups linked through a propyl group to the silicone atom (MPM, 2021b).

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for dimethylsiloxane, ethylene oxide block copolymer.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5. ENVIRONMENTAL FATE SUMMARY

Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is a large molecular weight block polymer for which very little environmental fate data exists. Silicone-based polymers can be attacked and hydrolysed under acidic or alkaline conditions. Trisiloxane-based polymers, such as dimethylsiloxane, ethylene oxide block copolymer (polysiloxane), are especially vulnernable as they can degrade outside neutral pH conditions over time (MPM, 2021b).

Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is not readily biodegradable. Copolymers of this type typically have a molecular weight greater than 1,000 g/mol. Based on this molecular weight, the substance is not expected to bioaccumulate (as concluded in the Categorization Results from the Canadian Domestic Substance List).

6. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No data on the environmental effects of the polymer were found. However, the high molecular weight of the substance is expected to negate or limit the bioavailability of the substance thus minimizing toxic effects on environmental receptors.

NICNAS has assessed dimethylsiloxane, ethylene oxide block copolymer (under generic CAS No. 68937-54-2) in an IMAP Tier 1 assessment and considers it a "polymer identified as a low concern to the environment."[1]. As a polymer of low concern, the substance is not expected to bioaccumulate or bioconcentrate. It may sorb to sediments and soil; however, it is not expected to exhibit toxicity to environmental receptors.

B. Aquatic Toxicity

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is not readily biodegradable; thus, it meets the screening criteria for persistence.

Dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is a high molecular weight polymer that is not expected to bioaccumulate. Thus, the substance does not meet the screening criteria for bioaccumulation.

There are no acute or chronic toxicity studies on dimethylsiloxane, ethylene oxide block copolymer (polysiloxane). However, as a polymer of low concern, it is not expected to exhibit toxicity to environmental receptors. Thus, dimethylsiloxane, ethylene oxide block copolymer (polysiloxane)does not meet the screening criteria for toxicity.

The overall conclusion is that dimethylsiloxane, ethylene oxide block copolymer (polysiloxane) is not a PBT substance.

[1] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.
https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=68937-54-2

B. Other Characteristics of Concern

No other characteristics of concern were identified for dimethylsiloxane, ethylene oxide block copolymer (polysiloxane).

8. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Dimethylsiloxane, ethylene oxide block copolymer	27306-78-1	Not a PBT	No	Yes	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = Bioaccumulative

P = persistent

T = toxic

9. REFERENCE, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

DISODIUM METASILICATE

This dossier on disodium metasilicate presents the most critical studies pertinent to the risk assessment of disodium metasilicate in its use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the OECD-SIDS documents on Soluble Silicates, which includes disodium metasilicate (OECD, 2004); and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Disodium metasilicate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Disodium metasilicate is a crystalline silicate that is readily solubilized in water. In the solubilized form, it is indistinguishable from solubilized amorphous silicates (e.g., sodium silicate). Upon dissolution in water, disodium metasilicate forms sodium ions (Na^+) and molecular speciation of silicates.

Disodium metasilicate is an inorganic substance and therefore not amenable to biodegradation. It is not expected to bioaccumulate. It is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium oxosilanebis(olate)

CAS RN: 6834-92-0

Molecular formula: Na_2O_3Si

Molecular weight: Not applicable; disodium metasilicate is comprised of infinite chains of Na2O3Si units of variable length.

Molar ratio: 1.0.

Synonyms: Disodium metasilicate; Disodium oxosilanebis(olate); sodium metasilicate; sodium metasilicate anhydrous; silicic acid, disodium salt (anhydrous); sodium metasilicate pentahydrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Disodium Metasilicate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless or white solid	-	ECHA
Melting Point	1089 °C (pressure not indicated)*	2	ECHA
Boiling Point	Not applicable	-	ECHA
Density	2,610 kg/m^3 (temperature not indicated)	2	ECHA
Vapour Pressure	0.00103 kPa @ 1175 °C	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	ECHA
Water Solubility	210 g/L @ 20 °C	2	ECHA
Dissociation Constant (pKa)	9.9, 11.8, 12 @ 30 °C	2	ECHA
Viscosity	Not applicable	-	ECHA

*Anhydrous form of disodium metasilicate

Sodium silicate is produced by fusing high purity quartz sand (SiO_2) and sodium carbonate or soda (Na_2CO_3) at temperatures of 1,300 to 1,500°C. The product that is formed is an amorphous glass that can be dissolved in water to produce silicate solutions. Various products of sodium silicate are obtained by varying the mixing ratio of quartz and soda. Sodium silicates are therefore characterized primarily by the SiO_2 to Na_2O ratio, or molar ratio (MR). Soluble silicates are generally not distinct stoichiometric chemical substances (with a specific chemical formula and molecular weight), but glasses or aqueous solutions of glasses (OECD, 2004).

Disodium metasilicate is a crystalline silicate, produced exclusively in the sodium form, by controlled crystallization of silicate solutions. The MR of disodium silicate is 1.0. Disodium metasilicate can be prepared in anhydrous form, or with water of crystallization as the penta- or nonahydrate (OECD, 2004).

Disodium metasilicate is readily solubilized in water. In the solubilized form, it is indistinguishable from solubilized amorphous silicates (e.g., sodium silicate). Upon dissolution in water, disodium metasilicate forms sodium ions (Na^+) and molecular speciation of silicates. Depending on both pH and concentration the respective solutions contain varying proportions of monomeric tetrahydral ions, oligomeric linear or cyclic silicate ions (OECD, 2004).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for disodium metasilicate.

NICNAS has assessed disodium metasilicate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Disodium metasilicate readily dissolves in water to sodium ions (Na^+) and molecular speciation of silicates. Dissolved silica from commercial soluble silicates is indistinguishable from natural dissolved silica. Silica (SiO_2) represents about 59% of the elemental composition of the earth's crust. Similar percentages are obtained for many sediments and soils (Jackson, 1964). Compounds of silicon and oxygen are ubiquitous in the environment; it is present in inorganic matter, like minerals and soils and in organic matter.

Silica is found in all natural waters and the median values in the U.S. were reported to be 17 mg SiO_2/L for ground waters and 14 mg SiO_2/L for streams (Davis, 1964). The world-wide concentration in rivers is 13 mg SiO_2/L (Edwards and Liss, 1973).

Disodium metasilicate is an inorganic substance and therefore not amenable to biodegradation. It is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Disodium metasilicate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on disodium metasilicate.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=6834-92-0

Table 3 Acute Aquatic Toxicity Studies on Disodium Metasilicate and Sodium Silicate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rario (previous name Brachydanio rerio)	96-hr LC_{50}	210	2	ECHA; OECD, 2004
Brachydanio rerio	96-hour LC_{50}	1,108*	2	ECHA; OECD, 2004
Oncorhynchus mykiss	96-hour LC_{50}	260 – 310*	2	ECHA; OECD, 2004
Daphnia magna	48-hour EC_{50}	1,700*	2	ECHA; OECD, 2004
Scenedesmus subspicatus	72-hour EC_{50}	207 (biomass)* >345.4 (growth rate)*	2	ECHA; OECD, 2004

*sodium silicate (CAS No. 1344-09-8)

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

There are no studies on disodium metasilicate or sodium silicate. A honeybee acute contact toxicity study according to (USEPA, 2012) has been conducted on AgSil™ 25 potassium silicate solution (29.1% potassium silicate in water). The 48-hr LD_0 was 25 µg/animal and the 48-hr LD_{50} was 25 µg/animal (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Disodium metasilicate is an inorganic compound that dissociates completely to sodium and silicate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and silicate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic compound.

Sodium and silicate ions are essential to all living organisms and is ubiquitous in the environment. Therefore, disodium metasilicate is not expected to bioaccumulate.

No chronic toxicity data exist on disodium metasilicate; however, the acute E(L)C50 values for disodium metasilicate and read-across substance sodium silicate are >1 mg/L in fish, invertebrates and algae. Therefore, disodium metasilicate does not meet the screening criteria for toxicity.

The overall conclusion is that disodium metasilicate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for disodium metasilicate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Disodium metasilicate	6834-92-0	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilograms per cubic metre

kPa	kilopascal
L	litre
LC	lethal concentration
LD	lethal dose
m	metre
mg/L	milligrams per litre
MR	molar ratio
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
USEPA	United States Environmental Protection Agency
µg	micrograms

DISODIUM OCTABORATE TETRAHYDRATE

This dossier presents the most critical studies pertinent to the risk assessment of disodium octaborate tetrahydrate in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion –Disodium octaborate tetrahydrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1. BACKGROUND

Disodium octaborate tetrahydrate is a boron compound. Boron compounds (including boron oxides, boric acid, boron minerals) have a wide range of applications in industry (e.g. manufacture of glass, fibreglass and porcelain enamels, and precursors for chemical manufacture), agriculture (e.g. fertilisers, herbicides and insecticides), and in household settings (e.g. flame retardants and detergents) and personal care products. Borate salts are commonly used in coal seam gas applications internationally (NICNAS, 2019).

Disodium octaborate tetrahydrate as a natural element is not degradable. It is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

Disodium octaborate tetrahydrate has low acute and chronic toxicity to aquatic organisms.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): disodium octaborate

CAS RN: 12008-41-2

Molecular formula: $Na_2B_8O_{13}{\cdot}4H_2O$

Molecular weight: 412.4 g/mol

Synonyms: boron sodium oxide tetrahydrate; boric acid, disodium salt, tetrahydrate; disodium octaborate tetrahydrate

3. PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for disodium octaborate tetrahydrate are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Disodium Octaborate Tetrahydrate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, odorless, crystalline powder	1	ECHA
Melting Point	>1,000°C (pressure not provided)	1	ECHA
Boiling Point	Not Applicable	-	ECHA
Density	1874 kg/m^3 @ 20°C	1	ECHA
Vapor Pressure	9.9 x 10^{-17} Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	Not Applicable, substance is inorganic	-	ECHA
Water Solubility	223.65 g/L @ 20°C	1	ECHA
Dissociation Constant (pKa)	8.94 @ 20°C	1	ECHA

Boron is almost exclusively found in the environment in the form of boron-oxygen compounds, which are often referred to as borates. The high strength of the B-O bond relative to those between boron and other elements makes boron oxide compounds stable compared to nearly all non-oxide boron materials. Indeed, the B-O bond is among the strongest found in the chemistry of naturally occurring inorganic substances (ECHA).

In the environment, the chemicals in this group will dissociate and/or hydrolyse to release boron as boric acid [B(OH) (also formulated as H BO)] and/or borate anions (NICNAS, 2019).

Exposure to borates are often expressed in terms of boron (B) equivalents based on the fraction of boron in the source substance on a molecular weight basis. The B equivalents used are a generic designation rather than a designation of the element boron. The factor for converting disodium octaborate tetrahydrate to B-equivalents is 0.2096.

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for disodium octaborate tetrahydrate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5. ENVIRONMENTAL FATE PROPERTIES

A. Summary

Disodium octaborate tetrahydrate as a natural element is not degradable. It is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

B. Partitioning

Chemicals in this group will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions. Boric acid is highly water soluble and it tends to remain in surface waters. Although some partitioning from water to soil and sediment does occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5 to9.0) (NICNAS, 2019).

C. Biodegradation

Degradation is not applicable to inorganic borates, such as disodium octaborate tetrahydrate. It is not subject to hydrolysis, photodegradation, or biodegradation (ECHA). Inorganic borates are subject to chemical transformation processes (adsorption, complexation, precipitation, fixation) once released into the environment (ECHA).

D. Environmental Distribution

The Kp value for disodium octaborate tetrahydrate was calculated as the median of all measured Kp values from the GEMAS project (Geochemical Mapping of Agricultural and Grazing Land Soil project): 2.19 L/kg dry weight (ECHA) [Kl. Score = 2]. The chemistry of boron in soils and aquatic systems is simplified by the absence of oxidation- reduction reactions or volatilization. Redox processes can mobilize Fe oxides and Mn oxides, which may lead to a release of boron in aquatic systems. Generally, sediments are characterised with higher pH values than the soil matrix, which increases the boron sorption capacity (ECHA).

If released to soil, based on this low Kp value, low vapour pressure and high water solubility, disodium octaborate tetrahydrate is considered relatively mobile in the environment, under certain conditions (ECHA).

E. Bioaccumulation

The WHO review of boron (WHO, 1998) noted that "highly water soluble materials are unlikely to bioaccumulate to any significant degree and that borate species are all present essentially as un-dissociated and highly soluble boric acid at neutral pH". A BCF of <0.1 was reported in Chinook salmon fed boron-supplemented diets for 60 to 90 days (Hamilton and Wiedmeyer, 1990).

6. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Disodium octaborate tetrahydrate has low acute and chronic toxicity to aquatic organisms.

B. Aquatic Toxicity

In ecotoxicological tests for boron, the exposure concentrations are expressed as boron equivalents i.e. mg B/L. This is because boric acid and borate salts will have the same boron speciation when dissolved in environmental matrices. Therefore, in the following sections toxicological values are given as mg B/L regardless of the form of boron that was tested.

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on disodium octaborate tetrahydrate.

Table 4: Acute Aquatic Toxicity Studies on Disodium Octaborate Tetrahydrate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fathead minnow	96-hr LC_{50}	79.7	2	ECHA
Stonefly, Shortwing snowfly	96-hr LC_{50}	476	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	52.4 mg B/L	1	ECHA

Chronic Studies

Long-term effects (LC_{10}) on freshwater fish ranged from 3.5 to 47 mg B/L. Adequate long-term LC10 of 21.6 mg B/L was found for the fresh water fish *P. promelas* in a study according to EPA OPPTS 850.1400 (ECHA) [Kl. Score = 2].

Long-term effects (LC10/NOEC) on reproduction on freshwater vertebrates ranged from 6.6 to 32 mg B/L based on several well-accepted guideline studies (ECHA) [Kl. Scores =1 or 2].

Boric acid has been evaluated for its toxicity towards the fresh water alga *Pseudokirchneriella subcapitata* (formerly *Selenastrum capricornutum*) in an Alga growth inhibition test according to OECD 201 under GLP requirements. The exposure duration was 72 hours under static conditions. The NOEC growth rate determined from the study was 17.5 mg B/L (ECHA) [Kl. Score = 1].

The ANZG water quality guideline (2021) derived a very high reliability default guideline value (DGVs) for (dissolved) boron in freshwater from 22 chronic (long-term) toxicity data, comprising eight fish, two amphibians, three crustaceans, one bivalve, three macrophytes, one green microalga, three diatoms and one blue–green alga. The summary of representative data used by ANZG to develop a water quality guideline for boron is presented in Table 5 below. These values are noted to be consistent with those reported in ECHA. Additional chronic aquatic toxicity data is found in the ANZG Technical Brief (ANZG, 2021).

Table 5: Chronic Aquatic Toxicity Studies on Boron[1]

Test Species	Endpoint	Results (mg/L)
Danio rerio	34-day NOEC (Biomass)	1.8
*Pimephales promela*s	32-day NOEC (Mortality)	11
Daphnia magna	14-day NOEC (Reproduction)	2.4
Pseudokirchneriella subcapitata	4-day NOEC (Growth)	2.8

1 - The DGVs are based on toxicity data for boron as either boric acid, H_3BO_3 (CAS 10043-35-3), or borax, $Na_2B_4O_710H_2O$ (CAS 1303-96-4), in freshwater.

In the chronic toxicity data set, fish sensitivity to boron ranged from the least sensitive species in the dataset (*Melanotaenia splendida*, LC10 102 mg/L) to the third most sensitive species in the dataset (*Danio rerio*, NOEC 1.8 mg/L). Of the crustaceans, *D. magna* was best represented in the literature, with 18 published NOEC values (ranging from 2.4 mg/L to 29 mg/L) for six different endpoints from six different publications. The final NOEC of 2.4 mg/L used in the DGV derivation was lower than that for *C. dubia* (NOEC 5.6 mg/L) and for the amphipod *H. azteca* (NOEC 6.6 mg/L).For *P. subcapitata*, there were three separate studies available with toxicity data for boron. The toxicity values from these studies ranged from a NOEC of 2.8 mg/L to a NEC of 27 mg/L, varying with endpoint, duration and test medium used. Boron was least toxic to *P. subcapitata* when tested in algal growth medium with added $NaHCO_3$, suggesting that carbonate addition may have influenced boron toxicity. Therefore, although NECs are preferred to NOECs or EC10s (Warne et al. 2018), in this instance, a reliable NOEC of 2.8 mg/L was the most sensitive toxicity value for *P. subcapitata* (ANZG, 2021).

C. Terrestrial Toxicity

Ecotoxicological tests with plants and soil invertebrates have recorded modest chronic toxicity values (NOECs/ECs) in the range of 15.3 to 84.0 and 5.2 to 315 mg total B/kg, respectively (ECHA, 2008). However, to predict the potential toxicity of boron to plants and soil organisms, measuring the total boron concentration may be unsuitable. Instead, potential toxicity is better predicted using boron concentrations in the soil solution (extractable boron) (Mertens, et al., 2011). In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron (NICNAS, 2019).

The avian toxicity studies conducted on disodium octaborate and boric acid are presented in Table 6.

Table 6: Avian Toxicity Studies on Disodium Octaborate and Boric Acid

Test Species	Test Substance	Endpoint	Results	Klimisch score	Reference
Mallard duck	Disodium octaborate	dietary LC_{50}	>2,100 mg B/kg food	1	EU, 2007
Bobwhite quail	Boric acid	dietary LC_{50}	>983 mg B/kg food	1	EU, 2007
Bobwhite quail	Disodium octaborate	Oral gavage LD_{50}	>527 mg B/kg bw	4	EU, 2007
Bobwhite quail	Disodium octaborate	dietary LC_{50}	>2,100 mg B/kg food	1	EU, 2007

7. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Disodium octaborate tetrahydrate is an inorganic compound that dissociates completely to boric acid and the borate anion in aqueous media. Biodegradation is not applicable to these inorganic compounds; both boric acid and borate are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to disodium octaborate tetrahydrate.

Disodium octaborate tetrahydrate is a water-soluble substance that is not expected to bioaccumulate. Limited data indicate that bioaccumulation (BCF values are low) is not significant in aquatic and terrestrial food chains. Thus, it does not meet the criteria for bioaccumulation.

The chronic toxicity data on disodium octaborate tetrahydrate has a NOEC > 0.1 mg/L. Thus, disodium octaborate tetrahydrate does not meet the criteria for toxicity.

The overall conclusion is that disodium octaborate tetrahydrate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for disodium octaborate tetrahydrate.

8. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Disodium Octaborate Tetrahydrate	12008-41-2	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 1 - Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry

kg	kilograms
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NEC	no effect concentration
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

DIUTAN (CAS No. 595585-15-2)

DIUTAN GUM (CAS No. 125005-87-0)

This dossier on diutan and diutan gum presents the most critical studies pertinent to the risk assessment of these substance in its use in hydraulic fracturing fluids. Diutan (CAS No. 595585-15-2) can also be referred to as diutan gum (CAS No. 125005-87-0). This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained for diutan gum from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Diutan and diutan gum are classified as **tier 1** chemicals and requires a hazard assessment only.

1 BACKGROUND

Diutan/Diutan gum is a natural high-molecular-weight gum produced by carefully controlled aerobic fermentation. The repeating unit is composed of a six-sugar unit. The backbone is made up of d-glucose, d-glucuronic acid, d-glucose, and l-rhamnose, and the side chain of two l-rhamnose. When added to cement grouts, diutan/diutan gum exhibits a shear-thinning behaviour. At low shear rates, the grout shows a high apparent viscosity resulting from entanglement and intertwining of the polymer, whereas at high shear rates the viscosity decreases because of the alignment of the polymer along the direction of the flow, thus enhancing fluidity.

Diutan/diutan gum is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil. Diutan/diutan gum is of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Names (IUPAC): (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal (2R,3S,4R,5R)-2,3,4,5,6-pentahydroxyhexanal (2S,3S,4S,5R)-2,3,4,5-tetrahydroxy-6-oxohexanoic acid acetic acid calcium dihydride hydrate magnesium dihydride potassium hydride sodium hydride

CAS RN: 125005-87-0

Molecular formula: $C_{20}H_{46}CaKMgNaO_{21}$

Molecular weight: Not applicable as substance is a UVCB.

Synonyms: Diutan gum; S 657; S-657 Gum; GEOVIS XT; GEOVIS XTL; KELCO-CRETE DG

Chemical Name (IUPAC): D-glucuronic acid, polymer with 6-deoxy L-mannose and D-glucose, acetate, Ca Mg K Na salt

CAS RN: 595585-15-2

Molecular formula: $(C_6H_{12}O_6.\ C_6H_{12}O_5.\ C_6H_{10}O_7)x.C_2H_4O_2.$ xCa.xK.xMg.xNa

Molecular weight: Not applicable as substance is a UVCB.

Synonyms: Diutan; D-Glucurono-D-gluco-6-deoxy-L-mannan, acetate, calcium magnesium potassium sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for diutan gum are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Diutan Gum (CAS No. 125005-87-0)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Off white solid powder	1	ECHA
Melting Point	No melting point was determined. Test substance decomposed at >175°C.	2	ECHA
Boiling Point	No data	-	-
Density	1430 Kg/m^3 @ 20°C	2	ECHA
Vapor Pressure	~0.1 kPa @ 25 °C	-	NICNAS, 2010
Partition Coefficient (log K_{ow})	-3.56 @ 20°C	2	ECHA
Water Solubility	40 g/L @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for diutan or diutan gum.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Diutan/diutan gum is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Biodegradation

A GLP-compliant study conducted in accordance with OECD guideline was available. The test material (diutan gum) attained 95% degradation after 28 days and satisfied the 10-day window validation criterion, whereby 60% degradation must be attained within 10 days of the degradation rate exceeding 10%. The test material can therefore be considered to be readily biodegradable under strict terms and conditions of the OECD guideline 301B. [Kl. Score = 1] (ECHA).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for diutan/diutan gum. Based on the low experimentally determined log K_{ow} (-3.56) value, the substance has a low potential to adsorb to soil and will be highly mobile in soil.

D. Bioaccumulation

No experimental data are available for diutan/diutan gum. Based on the low log K_{ow} (-3.56), the potential for bioaccumulation is low.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Diutan is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 presents the results of acute aquatic toxicity studies on diutan/diutan gum.

Table 3 Acute Aquatic Toxicity Studies on Diutan Gum

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss (Rainbow Trout)	96-h LC_{50}	100	1	ECHA
Daphnia magna	48-h LC_{50}	>100	1	ECHA
Desmodesmus subspicatus (previous name: Scenedesmus subspicatus)	72-h EC_{50}	>100 (growth rate and biomass)	1	ECHA

Chronic Studies

No data are available.

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Diutan/diutan gum is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Bioaccumulation of diutan/diutan gam is not expected to occur based on it log K_{ow} value of -3.56 . Thus, diutan/diutan gum does not meet the screening criteria for bioaccumulation.

No chronic toxicity data is available. The $E(L)C_{50}$ values from the acute aquatic toxicity studies on diutan/diutan gum are >1 mg/L. Thus, diutan/diutan gum does not meet the criteria for toxicity.

Therefore, diutan/diutan gum is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for diutan/diutan gum.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Diutan	595585-15-2	Not a PBT	No	No	No	No	No	No	1	No data	1
Diutan Gum	125005-87-0	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 – PBT Assessment based on PBT Framework.

2 – Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

DoEE. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2010). National Industrial Chemicals Notification and Assessment Scheme (NICNAS) Full Public Report: Diutan Gum. File SN/20. May 2010.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
GLP	Good Laboratory Practice
IUPAC	International Union of Pure and Applied Chemistry
Kl	Klimisch
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre

NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

ETHYLENE GLYCOL MONOBUTYL ETHER

This dossier on ethylene glycol monobutyl ether (EGBE) presents the most critical studies pertinent to the risk assessment of EGBE in its use in drilling muds and hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on EGBE, and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – EGBE is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

EGBE is readily biodegradable. It is not expected to bioaccumulate. EGBE has a low tendency to bind to soil or sediment. EGBE is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-Butoxyethanol

CAS RN: 111-76-2

Molecular formula: $C_6H_{14}O_2$

Molecular weight: 118.18 g/mol

Synonyms: Ethylene glycol monobutyl ether, EGBE, 2-butoxyethanol, butyl cellosolve, butyl glycol, glycol monobutyl ether

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of EGBE

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	A colourless liquid. Odour is mild, ether-like, and slightly rancid.	2	ECHA
Melting Point	-74.8°C @ 101.3 kPa	2	ECHA
Boiling Point	171 – 171.5°C @ 101.3 kPa	2	ECHA
Density	900 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	80 Pa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	0.81 @ 20°C	1	ECHA
Water Solubility	900 g/L @ 20°C (fully soluble)	2	ECHA

Property	Value	Klimisch score	Reference
Dissociation Constant (pKa)	15 @ 20°C	2	ECHA
Viscosity	3.28 mPa.s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for EGBE.

Based on an assessment of environmental hazards, NICNAS identified EGBE as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

EGBE is readily biodegradable. It is not expected to bioaccumulate. EGBE has a low tendency to bind to soil or sediment.

B. Biodegradation

EGBE was considered readily biodegradable in an OECD 301B test. Degradation was 90.4% after 28 days; the 10-day window was met (ECHA) [Kl. score = 2]. Results from another OECD 301B test showed 63% and 74-75% degradation after 10 and 28 days, respectively (ECHA) [Kl. score = 2]. An OECD 301 D test showed 67-75% degradation after 15 days and 73-77% after 28 days (ECHA) [Kl. score = 2]. In a Zahn-Wellen (OECD 302B test), degradation of EGBE was 95% after 8 days, measured as DOC removal (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for EGBE. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 7.624 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 2.823 L/kg.

Based upon these K_{oc} values, if released to soil, EGBE is expected to have low potential for adsorption and a high potential for mobility. If released to water, based on its K_{oc} and high water solubility values, EGBE is likely to remain in water and not adsorb to sediment.

D. Bioaccumulation

No bioconcentration studies have been conducted on EGBE. EGBE is not expected to bioaccumulate based on the experimental log K_{ow} of 0.81 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

EGBE is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on EGBE.

Table 3 Acute Aquatic Toxicity Studies on EGBE

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	1,464	2	ECHA
Pimephales promelas	96-hour LC_{50}	2,137	2	ECHA
Pimephales promelas	96-hour LC_{50}	1,700	2	ECHA
Pimephales promelas	96-hour LC_{50}	1,580	2	ECHA
Lepomis machrochirus	96-hour LC_{50}	1,490	2	ECHA
Salmo gairdneri	96-hour LC_0	>1,000	2	ECHA
Daphnia magna	48-hour EC_{50}	1,800	2	ECHA
Daphnia magna	48-hour EC_{50}	1,815	2	ECHA
Daphnia magna	48-hour EC_{50}	881 (cited) 1,100 (recalculated by ECHA)	2	ECHA
Daphnia magna	48-hour EC_{50}	2,650	2	ECHA
Pseudokirchneriella subcapitata	72-hour EC_{50} NOEC	911 (biomass) 88	1	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Selenastrum capricornutum	72-hour EC_{50} NOEC	720 (biomass) 280	2	ECHA

Chronic Studies

A 21-day fish (*Brachydanio rerio*) study was conducted to examine the potential for endocrine disrupting effects; the study design was based on the OECD TG 204. The NOEC was >100 mg/L (ECHA) [Kl. score = 2].

The NOEC from a 21-day *Daphnia* reproduction study was 100 mg/L (ECHA) [Kl. score = 1].

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

EGBE is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 0.81, EGBE does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on EGBE show NOECs of >0.1 mg/L. Thus, EGBE does not meet the screening criteria for toxicity.

The overall conclusion is that EGBE is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for EGBE.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
EGBE	111-76-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2017). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency

EGBE	ethylene glycol monobutyl ether
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg/L	milligrams per litre
mm^2/s	square millimetres per second
mPa.s	millipascal second
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	screening information data set
TG	test guideline

ETHYLENE OXIDE/PROPYLENE OXIDE COPOLYMER (CAS NO. 9003-11-6)
ETHYLENE OXIDE/PROPYLENE OXIDE COPOLYMER (CAS NO. 9082-00-2)

This dossier on ethylene oxide/propylene oxide copolymer (EO/PO copolymer) presents the most critical studies pertinent to the risk assessment of EO/PO copolymer in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – EO/PO copolymer is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

EO/PO copolymer is a group of polymers that can vary in molecular weight (size). They are non-volatile and vary in water solubility. EO/PO copolymers are either readily biodegradable or inherently biodegradable and are not expected to bioaccumulate. EO/PO copolymers are practically acutely non-toxic to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Oxirane, methyl-, polymer with oxirane

CAS RN: 9003-11-6

Molecular formula: $(C_3H_6O.C_2H_4O)_x$-

Molecular weight: Variable

Synonyms: ethylene oxide, propylene oxide block polymer; poloxalene; poloxamer; polyethylene glycol, propoxylated; polyethylene-polypropylene glycol; polyoxyethylene-oxy-propylene; oxirane, 2-methyl-, polymer with oxirane; oxirane, methyl-, polymer with oxirane

Chemical Name (IUPAC): Oxirane, methyl-, polymer with oxirane, ether with 1,2,3-propanetriol (3:1)

CAS RN: 9082-00-2

Molecular formula: $C_3H_8O_3.3(C_3H_6O.C_2H_4O)_x$-

Molecular weight: Variable

Synonyms: Ethylene oxide-propylene oxide copolymer ether with glycerol (3:1); ethylene oxide-propylene oxide copolymer glycerol ether; glycerol, ethylene oxide, propylene oxide polymer; glycerol poly(oxyethylene, oxypropylene) ether; propylene oxide ethylene oxide polymer, ether with glycerol (3:1); glycerol, propylene oxide, ethylene oxide polymer

3 PHYSICO-CHEMICAL PROPERTIES

The physico-chemical properties of the EO/PO copolymers are listed in Table 1.

Table 1 Overview of the Physico-chemical Properties of Selected EO/PO Copolymers (CIR, 2008)

Properties	Poloxamer 124	Poloxamer 188	Poloxamer 407
Avg. molecular weight (g/mol)	2090-2360	7680-9510	9840-14600
Description	Colourless liquid	White solid	Solid
Wt. % oxyethylene	46.7 ± 1.9	81.8 ± 1.9	73.2 ± 1.7
Melting point (°C)	16	52	56
Solubility	Soluble in water	Soluble in water	Soluble in water

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for EO/PO copolymer.

NICNAS has assessed poloxalene (CAS No. 9003-11-6) in an IMAP Tier 1 assessment and considers it a polymer of low concern[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

No studies are available.

The following information is from the Dow Chemical Company's Product Safety Assessment document on their EO/PO copolymer products with CAS RN 9003-11-6 and 53637-25-5 (Dow, 2014):

"Polyglycol EP Series Polymers are non-volatile (do not evaporate) and vary in water solubility. If released to water or soil, they would tend to remain in and be transported with the surface or ground water to which they are emitted, and will be adsorbed to soil and sediment particles. Polyglycol EP Series Polymers are unlikely to persist in the environment, as all products are known or expected to be either readily biodegradable (>65% biodegraded in 28 days per OECD 301F test) or inherently biodegradable according to Organisation for Economic and Co-operation and Development (OECD) test guidelines. As such, these products will be efficiently removed during treatment in biological wastewater-treatment facilities."

"These products are not expected to accumulate in the food chain (low bioconcentration potential)."

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Aquatic Toxicity

No studies are available.

The following information is from the Dow Chemical Company's Product Safety Assessment document on their EO/PO copolymer products with CAS RN 9003-11-6 and 53637-25-5 (Dow, 2014):

"[EO/PO copolymers] are practically non-toxic to aquatic organisms (LC_{50}/EC_{50} >100 mg/L for the most sensitive species tested) on an acute basis."

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

EO/PO copolymers are either readily biodegradable or inherently biodegradable; thus, they do not meet the screening criteria for persistence.

EO/PO copolymers are expected to have high molecular weights and are not expected to be bioavailable. Thus, these copolymers do not meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on the EO/PO copolymers. However, the acute EC_{50} on these copolymers are >0.1 mg/L in aquatic organisms based on information from Dow Chemical's Product Safety Assessment (Dow, 2014). EO/PO copolymers also have a high molecular weight and are not expected to be bioavailable. Thus, they do not meet the screening criteria for toxicity.

The overall conclusion is that EO/PO copolymers are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for EO/PO copolymer.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
EO/PO Copolymer	9003-11-6	Not a PBT	No	Yes	No	No	No	No	1	1	1
EO/PO Copolymer	9082-00-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Cosmetic Ingredient Review (CIR). (2008). Safety Assessment of Poloxamers 101, 105, 108, 122, 123, 124, 181, 182, 183, 184, 185, 188, 212, 215, 217, 231, 234, 235, 237, 238, 282, 284, 288, 331, 333, 334, 334, 338, 401, 402, 403, and 407, Poloxamer 105 benzoate, and Poloxamer 182 dibenzoate as used in cosmetcs. Int. J. Toxicol. 27 (Supppl. 2): 93-128

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Dow Chemical Company. (Dow). (2014). Product Safety Assessment from Dow Chemical Company on their Polyglycol EP Series Polymers/FLUENT Brand Polyglycols/SYNALOX™ Fluids, revised June 5, 2014

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EO/PO	ethylene oxide/propylene oxide
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

ETHANOL, 2,2'-OXYBIS-, REACTION PRODUCTS WITH AMMONIA, MORPHOLINE DERIVATIVES RESIDUES

This dossier on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues presents the most critical studies pertinent to the risk assessment in its use in hydraulic fracturing fluids and water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is a UVCB with several compounds containing ionizable groups. It does not biodegrade but is not expected to bioaccumulate based on its low log K_{ow}. It is of low aquatic toxicity concern and is not a PBT.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-(2-hydroxyethoxy)ethan-1-ol; 2-[1-(morpholin-4-yl)ethoxy]ethan-1-amine; 2-{2-[bis(2-hydroxyethyl)amino]ethoxy}ethan-1-ol; 4-{2-[2-(morpholin-4-yl)ethoxy]ethyl}morpholine; morpholin-3-one

CAS RN: 68909-77-3

Molecular formula: $C_{36}H_{78}N_6O_{14}$

Molecular weight: 210.27 g/mol (Substance is a UVCB)

Synonyms: Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine product tower residues, Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues, Morpholine product tower residue.

3 PHYSICO-CHEMICAL PROPERTIES

The substance is defined as the residuum from the reaction of diethylene glycol and ammonia. It consists predominantly of morpholine-based derivatives such as [(aminoethoxy)ethyl]morpholine, [(hydroxyethoxy)ethyl]morpholine, 3-morpholinone, and 4,4'-(oxydi-2,1-ethanediyl)bis[morpholine].

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	dark brown liquid	2	ECHA
Melting Point	-20 °C @ 101.3 kPa	1	ECHA
Boiling Point	223 °C @ 101.3 kPa	1	ECHA
Density	1090 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	0.55 Pa @ 25 °C	1	ECHA
Partition Coefficient (log K_{ow})	0.565 @ 20 °C and pH=7	1	ECHA
Water Solubility	100 g/L @ 25 °C	1	ECHA
Viscosity	121.398 mm^2/s (static) @ 20 °C[1]	1	ECHA
Dissociation constant (pKa at 20°C)	The test substance is a UVCB with several compounds containing ionizable groups a single pKa cannot be defined.	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] Dynamic values in mPa s not available

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is inherently biodegradable. It is not expected to bioaccumulate nor is it anticipated to sorb to soils or sediment due to its high water solubility and low log K_{ow}.

B. Partitioning

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is highly soluble in water. Based upon a Henry's Law constant of 1.02 x 10^{-3} Pa*m³/mol, it is expected to have a low potential to volatilise from water and moist soil surfaces. However, it is expected to volatilise from dry soil surfaces based upon its vapour pressure. After evaporation or exposure to air, the substance will be rapidly degraded by photochemical processes (ECHA).

Hydrolysis is not expected. The assessment of hydrolytic stability of the substance was carried out according to the EU Method C.7. Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues was determined to be hydrolytically stable at pH 4, 7 and 9, with estimated half-lives greater than 1 year at 25°C (ECHA) [Kl. Score = 1].

C. Biodegradation

Two key studies are available and used to conclude on the ready biodegradability of the substance in an aerobic aqueous medium. Both studies are given a Klimisch score of 1 and were conducted under GLP. The first study (Clarke, 2010 - report 41003975) is carried out according to the OECD guideline 301B (CO2 evolution test), EC Method C.4-C. After 28 days, the observed biodegradation was 21% and the test substance is regarded as not readily biodegradable. The second study (Clarke, 2010 - report 41003980) is an enhanced biodegradation test carried out according to the OECD guideline 301B (CO2 evolution test), EC Method C.4-C. After 28 days, the observed biodegradation was 15%, and after 42 days, the observed biodegradation was 18%. The test substance is regarded as not readily biodegradable [Kl Score = 1](ECHA) but can be considered inherently biodegradable

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is greater than 60 days (DoEE, 2017).

D. Environmental Distribution

Adsorption/desorption studies were performed according to the EU Method C.19. The adsorption coefficient (K_{oc}) of Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues was determined to range from <17.8 (test material concentration of 89.6%) to 141 (test material concentration of 10.4%) at pH 5.5 and <17.8 (test material concentration of 89.6%) to 29.8 (test material concentration of 10.4%) at pH 7.5. The different Koc values obtained at different pH values, might result from ionization. Overall, significant adsorption is not expected [Kl Score = 1](ECHA).

Based upon these K_{oc} values, if released to soil, the substance is expected to have high mobility. If released into water, based on its high water solubility and these K_{oc} values, the substance is not expected to adsorb to suspended solids and sediment in water; and, as noted earlier, will dissociate.

E. Bioaccumulation

The substance has a low potential for bioaccumulation. Based on the available information on the log K_{ow} of the major components of the mixture "ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues" (CAS 68909-77-3) ranging from -2.26 to 0.5 (see IUCLID chapter 4.7) and supported by a weight-of-evidence approach from experimental and additional calculated data, it can be concluded that significant accumulation in organisms is not to be expected [Kl Score = 1](ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues is of low acute toxicological concern to aquatic organisms. Details are provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 presents the results of acute aquatic toxicity studies on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues.

Table 3 Acute Aquatic Toxicity Studies on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hr LC_{50}	45	1	ECHA
Daphnia magna	48-hr EC_{50}	100	1	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	45	1	ECHA

Chronic Studies

No chronic studies are available. Chemical safety assessments have not indicated the need to investigate further the effects on fish or invertebrates. The acute-to-chronic ratio (ACR) as determined following the ECETOC Technical Report No. 93 (Aquatic Hazard Assessment II; ECETOC, 2003) shows that a long-term NOEC for fish of > 0.45 mg/L and for daphnids of > 1 mg/L is to be expected. Moreover, the results from short-term toxicity tests on fish, Daphnia and algae demonstrate that aquatic invertebrates are the most sensitive trophic level tested (ECHA) [Kl. Score = 2].

C. Terrestrial Toxicity

No studies were found. The substance is not readily biodegradable. However, as the log K_{oc} of the mixture components is below 3, a low adsorption potential is indicated. Therefore, binding to

sewage sludge is unlikely and as a consequence a transfer to the soil compartment is not expected. Therefore, no tests on terrestrial organisms were provided (ECHA).

7 CATEGORISATION AND OTHER CHARCTERSTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Although ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues exhibits limited degradation, it is not readily biodegradable according to the specifics of degradation testing. However, it is considered inherently biodegradable...

Bioaccumulation of ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is not expected to occur based on its low K_{ow}. Therefore, the substance does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity data available on ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues. The acute E(L)C_{50} values > 1 mg/L. Thus, ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine does not meet the criteria for toxicity.

The overall conclusion is that ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivatives residues	68909-77-3	Not a PBT	No	No	No[4]	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

4 – Substance is not readily biodegradable per testing guidelines. However, the degradation rate exhibited suggests it the substance is inherently biodegradable.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
CO2	Carbon dioxide
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	Dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mol	grams per mol
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal

L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

ETHANOL

This dossier on ethanol presents the most critical studies pertinent to the risk assessment of ethanol in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. Ethanol consumption in alcoholic beverages is out of the scope of this dossier. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ethanol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Ethanol is highly water soluble, readily biodegradable with low sorption potential and relatively low toxicity to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Ethanol

CAS RN: 64-17-5

Molecular formula: C_2H_6O

Molecular weight: 46.069 g/mol

Synonyms: Ethyl alcohol, grain alcohol, alcohol, methylcarbinol, ethyl hydroxide, ethyl hydrate, algrain, alkohol, anhydrol

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Ethanol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid with a mild odour.	2	ECHA
Melting point	-114°C @ 101.3 kPa	2	ECHA
Boiling point	78.2°C @ 101.3 kPa	2	ECHA
Density	789 kg/m^3 @ 20°C	2	ECHA
Vapour pressure	0.05726 Pa @ 19.6°C	2	ECHA
Partition coefficient (log K_{ow})	-0.35 @ 24°C	2	ECHA

Property	Value	Klimisch score	Reference
Water solubility	789 g/L @ 20°C	2	ECHA
Dissociation Constant (pKa)	15.8 @ 20°C	2	ECHA
Viscosity	1.17 mPa.s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ethanol.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Ethanol is readily biodegradable and not expected to bioaccumulate.

B. Partitioning

Ethanol is highly soluble in water. Based upon a Henry's Law constant of 0.33 Pa*m³/mol, it is expected to volatilise from water and moist soil surfaces. It is also expected to volatilise from dry soil surfaces based upon its vapour pressure. Vapour-phase ethanol will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 5 days (PubChem).

C. Biodegradation

Ethanol is readily biodegradable. The degradation of ethanol was approximately 74% and 84% (O_2 consumption) within 10 and 20 days, respectively, in a biodegradation test using a non-adapted domestic inoculum in a freshwater medium (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for ethanol. Using KOCWIN in EPISuite™ (USEPA, 2019), the estimated K_{oc} value from log K_{ow} of -0.35 is 2.199 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 1.045 L/kg. Thus, ethanol is not expected to sorb substantially to sediments or soil and has a high potential for mobility. If released into water, ethanol is also not expected to adsorb to suspended solids and sediment in water; and, as noted earlier, volatilisation is expected to be an important fate process (PubChem).

E. Bioaccumulation

There are no bioaccumulation studies on ethanol. Ethanol is not expected to bioaccumulate based on a log K_{ow} of -0.35 (ECHA).

6 ENVIRONMENTAL HAZARD ASSESSMENT

A. Summary

Acute aquatic toxicity ranges from 275 to 15,300 mg/L, depending on species and exposure durations. While chronic toxicity ranges from 9.6 to 250 mg/L.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on ethanol.

Table 3 Acute Aquatic Toxicity Studies on Ethanol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	15,300	2	ECHA
Pimephales promelas	96-hour LC_{50}	14,200	2	ECHA
Ceriodaphnia dubai	48-hour EC_{50}	5012	2	ECHA
Chlorella vulgaris	72-hour EC_{50}	275	2	ECHA

Chronic Studies

The 5-day NOEC to *Brachydanio rerio* in an OECD 212 embryo and sac-fry stage test is 250 mg/L (ECHA) [Kl. Score = 2].

The 10-day NOEC to *Ceriodaphnia dubia* in a *Daphnia* reproduction test is 9.6 mg/L (ECHA) [Kl. Score = 2].

The 72-hour EC_{10} to algae *Chlorella vulgaris* is 11.5 mg/L (ECHA) [Kl. Score = 2].

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Ethanol is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -0.35, ethanol does not meet the screening criteria for bioaccumulation.

The EC_{10} or NOEC values from the chronic aquatic toxicity studies on ethanol are >0.1 mg/L. The acute EC_{50} values for ethanol are >1 mg/L. Thus, ethanol does not meet the criteria for toxicity.

Therefore, ethanol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ethanol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Ethanol	64-17-5	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 – PBT Assessment based on PBT Framework.

2 – Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

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PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

USEPA. (2019). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system

KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

ETHYLENE GLYCOL

This dossier on ethylene glycol presents the most critical studies pertinent to the risk assessment of ethylene glycol in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ethylene glycol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Ethylene glycol is readily biodegradable, and it is not expected to bioaccumulate. Ethylene glycol has low potential to adsorb to soil and sediment. Ethylene glycol is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Ethane-1,2-diol

CAS RN: 107-21-1

Molecular formula: $C_2H_6O_2$ ($HOCH_2CH_2OH$)

Molecular weight: 62.07 g/mol

Synonyms: Ethylene glycol; ethane-1,2-diol; 1,2-ethanediol, 2-hydroxyethanol; monoethylene glycol; MEG; glycol alcohol; EG

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Ethylene Glycol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless and odourless syrupy liquid	2	ECHA
Melting Point	-13°C @ 101.3 kPa	2	ECHA
Boiling Point	197.4°C @ 101.3 kPa	2	ECHA
Density	1110 kg/m^3@ 20°C	2	ECHA
Vapour Pressure	12.3 Pa @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	-1.36 (calculated) @ 25°C	2	ECHA
Water Solubility	1000 g/L @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Viscosity	16.1 mPa.s @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ethylene glycol.

Based on an assessment of environmental hazards, NICNAS identified ethylene glycol as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Ethylene glycol is readily biodegradable, and it is not expected to bioaccumulate. Ethylene glycol has low potential to adsorb to soil and sediment.

B. Biodegradation

Ethylene glycol was readily biodegradable in an OECD 301A test. After 10 days, degradation was 90-100% (ECHA) [Kl. score = 1]. There was 97% degradation after 20 days in a BOD test; and 96% degradation after 28 days in an OECD 301D test (Waggy et al., 1994; OECD, 2004a,b) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

The aerobic degradation of ethylene glycol was measured from grab river water samples at 4, 8 and 20°C. At 20°C, ethylene glycol was completely degraded in three days in all river waters tested; at 8°C, degradation was complete within 14 days. Degradation at 4°C was substantially slower, with

degradation of <20% after 14 days in river samples with limited suspended matter and a starting concentration of 10 mg/L (Evans and David, 1974).

C. Environmental Distribution

No experimental data are available for ethylene glycol. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values from the molecular connectivity index (MCI) and from the log K_{ow} are 1 and 0.2239 L/kg, respectively.

Based upon these K_{oc} values, if released to soil, ethylene glycol is expected to have low potential for adsorption and a high potential for mobility. If released to water, based on its K_{oc} and high water solubility values, ethylene glycol is likely to remain in water and not adsorb to sediment. From the water surface, the substance will not evaporate into the atmosphere (ECHA).

D. Bioaccumulation

The calculated log K_{ow} for ethylene glycol is -1.36 (ECHA). The BCF for ethylene glycol in golden ide (*Leuciscus idus melanotus*) after three days of exposure was determined to be 10 (Freitag *et al.*, 1985). Bioaccumulation is not to be expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Ethylene glycol is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on ethylene glycol.

Table 3 Acute Aquatic Toxicity Studies on Ethylene Glycol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	>72,860	1	Pillard (1995)
Oncorhynchus mykiss	96-hour LC_{50}	22,810 24,591	2	OECD (2004a,b)
Daphnia magna	48-hour EC_{50}	>100	1	ECHA
Daphnia magna	48-hour EC_{50}	46,300	2	Gersich et al. (1986)
Ceriodaphnia dubia-affinis	48-hour EC_{50}	25,800 (20°C) 10,000 (24°C)	2	Cowgill et al. (1985)
Daphnia magna	48-hour EC_{50}	46,300 (20°C) 51,000 (24°C)	2	Cowgill et al. (1985)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Selenastrum capricornutum	96-hour IC_{50} NOEC	10,940 10,000	2	Pillard and DuFresne (1999)

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies conducted on ethylene glycol.

Table 4 Chronic Aquatic Toxicity Studies on Ethylene Glycol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	7-day NOEC	15,380	2	Pillard (1995)
Ceriodaphnia dubia	7-day NOEC (reproduction)	8,590	2	Pillard (1995)
Pseudokirchneriella subcapitata	72-hr NOEC	>100 *	2	ECHA

*Read-across to pentaethylene glycol (CAS No. 4792-15-8)

C. Terrestrial Toxicity

No guideline studies have been conducted on ethylene glycol.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Ethylene glycol is readily biodegradable and thus does not meet the screening criteria for persistence.

The measured BCF in fish is 10. Thus, ethylene glycol does not meet the criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on ethylene glycol are >0.1 mg/L. The acute EC_{50} values from the acute aquatic toxicity studies on ethylene glycol are >1 mg/L. Thus, ethylene glycol does not meet the criteria for toxicity.

The overall conclusion is that ethylene glycol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ethylene glycol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Ethylene Glycol	107-21-1	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BOD	biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second

NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

FATTY ACIDS, TALL-OIL, ETHOXYLATED

This dossier on fatty acids, tall-oil, ethoxylated (FAT) presents the most critical studies pertinent to the risk assessment of the substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Fatty acids, tall-oil, ethoxylated is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

FAT is a UVCB used to facilitate emulsification. This CAS RN is broadly defined as a complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. Tall oil fatty acids (TOFA), generally any product containing 90% or more fatty acids and 10% or less of rosin, have grown in annual volume ever since, until they amounted to 398.8 million pounds annual production in the United States in 1978. Crude tall oil is a byproduct of the Kraft process for producing wood pulp from pine wood. Crude tall oil is about 50% fatty acids and 40% rosin acids, the remainder unsaps and residues. Separative and upgrading technology involves: (a) recovery of the tall oil; (b) acid refining; (c) fractionation of tall oil; and occasionally (d) conversion to derivatives. TOFA of good quality and colour of Gardner 2 corresponds to above 97% fatty acids with the composition of 1.6% palmitic and stearic acid, 49.3% oleic acid, 45.1% linoleic acid, 1.1% miscellaneous acids, 1.2% rosin acids and 1.7% unsaponifiables.

The substance is biodegradable, may sorb to sediments, is not expected to bioaccumulate and is of low toxicity to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Fatty acids, tall-oil, ethoxylated

CAS RN: 61791-00-2

Molecular formula: $C_{(18-50)}H_{(34-98)}O_{(3-8)}$ (UVCB substance)

Molecular weight: (UVCB substance)

Synonyms: 2-[(10Z,13Z)-nonadeca-10,13-dienoyloxy]ethyl (10Z,13Z)-nonadeca-10,13-dienoate 2-hydroxyethyl (5Z,9Z,12Z)-octadeca-5,9,12-trienoate 2-hydroxyethyl (9Z)-octadec-9-enoate 2-hydroxyethyl (9Z,12Z)-octadeca-9,12-dienoate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Fatty acids, tall-oil, ethoxylated

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid.	2	ECHA
Melting point	-85°C @ 101.3 kPa	2	ECHA
Boiling point	Not available. During the heating process the test item began to change its state at approximately 172°C from liquid to highly viscous. This indicates a thermally caused change of the test item.	2	ECHA
Density	958 kg/m^3 @ 20°C	2	ECHA
Vapour pressure	The vapour pressure could not be determined.	2	ECHA
Partition coefficient (log K_{ow})	5.94 @ 25°C	-	-
Water solubility	The test item can be mixed with water up to a ratio of 3:7 (m (test item):m (water)).	-	-
Viscosity	58.0 mPa.s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for fatty acids, tall-oil, ethoxylated.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

There are no biodegradation data on FAT. However, data on structurally similar substances suggest FAT is biodegradable with potential to sorb to soils. It is not expected to readily bioaccumulate.

B. Biodegradation

Data on the ready biodegradability of fatty acids, tall oil, ethoxylated (> 1 < 2.5) (CAS 61791-00-2) are not available. Therefore, data on the ready biodegradability of the structurally related analogue substance fatty acids, tall oil, ethoxylated (EO 5) (CAS No. 9004-96-0) is used as read-across in accordance with Regulation (EC) No. 1907/2006, Annex XI, 1.5.

This read-across is justified because both target and source substance are structurally identical (ethoxylated oleic acid) except for the fact that the source substance is slightly higher ethoxylated (5 EO) than the target substance (1-2.5 EO). This difference might lead to a slightly lower water solubility of the target substance; however, since the solubility of both substances is rather high and not limiting the bioaccessibility of the substances to aquatic microorganisms, is not considered to influence the identical biodegradation behaviour of both substances. Both substances share the same functional groups and the same mode of action (baseline toxicity caused by the long lipophilic fatty acid chain). Thus, biotransformation can, with very high certainty, be assumed to be identical.

The test with the source substance was conducted according to OECD Guideline 301B, under GLP conditions (ECHA). Domestic, non-adapted activated sludge was exposed to the test substance for 28 days at 22°C, and biodegradation was measured by CO_2 consumption. After 28 days, the test substance reached a biodegradation of 90 - 100%.

Based on the results for the read-across substance, fatty acids, tall oil, ethoxylated (EO > 1 < 2.5) (CAS 61791-00-2) is considered to be readily biodegradable. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

One study investigating the adsorption/desorption behaviour of fatty acids, tall-oil, ethoxylated (CAS 61791-00-2) is available. The study was performed according to GLP and OECD guideline 121 (ECHA). Six different peaks were observed with log K_{oc} values ranging from < 1.8 to > 5.63. The two main components (> 85%) show log K_{oc} values > 4. Thus, the substance shows moderate capacity to sorb to sediments.

Thus, adsorption of fatty acids, tall-oil, ethoxylated to solid soil is expected with limited potential for mobility.

D. Bioaccumulation

The test substance consists of components with log K_{ow} values in the range of 5 to > 10 (KOWWIN v1.68) indicating a potential for bioaccumulation. However, due to rapid environmental biodegradation, metabolisation via enzymatic hydrolysis (monoesters and diesters) as well as sterical hindrance of crossing biological membranes (high molecular weight of diesters) a relevant uptake

and bioaccumulation in aquatic organisms is not expected. This is supported by low BCF values of < 100 L/kg wet weight (BCFBAF v3.01, Arnot-Gobas, including biotransformation, upper trophic) calculated for different components of the UVCB (mono- and diester EO1 to EO5). Thus, taking all information into account, the test substance is not considered to be bioaccumulative.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance is of low acute toxicity concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

There are no aquatic toxicity data on the substance are listed on Table 3.

Table 3 Acute Aquatic Toxicity Studies on Fatty acids, tall-oil, ethoxylated*

Test Substance	Test Species	Endpoint	Results (mg/L) [WAF]	Kl. score	Reference
Fatty acids, tall-oil, ethoxylated	*Danio rerio*	96-hour LL_{50}	>100	1	ECHA
Fatty acids, tall-oil, ethoxylated	*Daphnia magna*	48-hour LL_{50}	12.41	1	ECHA
Fatty acids, tall-oil, ethoxylated	*Pseudokirchnerella subcapitata*	72-hour LL_{50}	39.7	1	ECHA

*All studies used the water accommodated fractions (WAFs) of the test substance.

Chronic Studies

No chronic data were available

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

FAT was noted to be readily biodegradable. Thus, the substance is not expected to meet the screening criteria for persistence.

Modelling of a representative structure indicates FAT does not have the potential to bioaccumulate. Thus, FAT does not meet the screening criteria for bioaccumulation.

FAT did not exhibit substantial acute toxicity to fish, invertebrates or algae. Thus, FAT is not expected to meet the screening criteria for toxicity.

The overall conclusion is that FAT is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for fatty acids, tall-oil, ethoxylated.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Fatty acids, tall-oil, ethoxylated	61791-00-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	USEPA EPISuite module to estimate bioconcentration and bioaccumulation factors
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	European Commission
ECHA	European Chemicals Agency
EU	European Union
FAT	fatty acids, tall-oil, ethoxylated
g/L	grams per litre
GLP	good laboratory practice
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre

KOWWIN	USEPA program to estimate the organic carbon-normalised sorption coefficient for soil and sediment
kPa	kilopascal
L/kg	litres per kilogram
LL	Loading level
mg/L	milligram per litre
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TOFA	tall oil fatty acid
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction

FATTY ACID ESTER (CAS NO. 135800-37-2)

This dossier on fatty acid ester (CAS No. 135800-37-2) presents the most critical studies pertinent to the risk assessment of fatty acid ester (CAS No. 135800-37-2) in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Fatty acid ester is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Fatty acid ester is a UVCB substance. Fatty acid ester (CAS No. 135800-37-2) is readily biodegradable. This substance has a low potential to bioaccumulate. It is highly insoluble in water and has high adsorption potential; thus, sediment and soil are expected to be the main targets for environmental distribution. Fatty acid ester (CAS No. 135800-37-2) is of low acute concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Fatty Acid Ester (CAS No. 135800-37-2)

CAS RN: 135800-37-2

Molecular formula: $C_{16}H_{32}O_2$ to $C_{24}H_{48}O_2$

Molecular weight: 256 to 352 g/mol

Synonyms: Fatty acids, C8-16, 2-ethylhexyl esters, Fatty acids, C8-16(even numbered), 2-ethylhexyl esters

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Fatty Acid Ester (CAS No. 135800-37-2)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear, slightly yellow liquid	2	ECHA
Melting Point	-53 to -30°C (pressure not provided)	1	ECHA
Boiling Point	-	-	-
Density	870 kg/m^3 @ 20°C (calculated)	2	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	<0.029 Pa @ 20°C (calculated)	2	ECHA
Partition Coefficient (log K_{ow})	6.68 to 8.65* (calculated) (temperature not provided)	2	ECHA
Water Solubility	<0.00005 g/L @ 20°C (measured)	2	ECHA
Dissociation Constant (pKa)	No dissociation	-	ECHA
Viscosity	7.4 mPa.s @ 20°C	2	ECHA

*Calculated from KOWWIN v 1.67 in EPISuite™ v. 4.00 (USEPA, 2017). Due to the fact that this substance is a long-chain hydrocarbon which exceeds the applicability domain of KOWWIN, the value for log K_{ow} is reported with restrictions. The applicability domain covers log K_{ow} up to 10 (maximum), so these values should be given as log K_{ow} >10.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for fatty acid ester.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Fatty acid ester (CAS No. 135800-37-2) is readily biodegradable. This substance has a low potential to bioaccumulate. It is highly insoluble in water and has high adsorption potential; thus, sediment and soil are expected to be the main targets for environmental distribution.

B. Biodegradation

In an OECD 301 D test, 97% (2 mg/L) and >65% (5 mg/L) were degraded after 30 days, indicating that fatty acid ester (CAS No. 135800-37-2) is readily biodegradable (ECHA) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental studies are available on fatty acid ester (CAS No. 135800-37-2). Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values of the surrogate dodecanoic acid, 2-ethylhexyl ester from the molecular connectivity index (MCI) and from log K_{ow} are 79,726 and 200,032 L/kg, respectively (ECHA). [Kl. score = 2] When released to the environment, based on its insolubility in water along with these estimated K_{oc} values, the fatty acid esters are likely to partition to soil and sediment and be immobile.

D. Bioaccumulation

No experimental studies are available on fatty acid ester (CAS No. 135800-37-2). Using the BCFBAF module in EPISuite™, the estimated BCF of the surrogate dodecanoic acid, 2-ethylhexyl ester is 1,054 L/kg based on a regression based estimate and 39.76 L/kg based on the Arnot-Gobas model which includes biotransformation and upper trophic. There would be rapid metabolism of fatty acid esters (initial hydrolysis by carboxylesterases) and excretion of linear aliphatic fatty acid esters from fish. Thus, bioaccumulation is not expected (ECHA). [Kl. score = 2]

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Fatty acid ester (CAS No. 135800-37-2) is of low acute concern to aquatic organisms, at least in the range of its water solubility.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on fatty acid ester (CAS No. 135800-37-2).

Table 3 Acute Aquatic Toxicity Studies on Fatty Acid Ester (CAS No. 135800-37-2)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Zebrafish	96-hour LC_{50}	>10,000*	2	ECHA
Daphnia magna	48-hour EC_{50}	>100** >100 (filtered test solution)[1]	1	ECHA
Daphnia magna	48-hour EL_{50}	>100 (WAF)	1	ECHA
Scenedesmus subspicatus	72-hour EC_{50}	<100 >100 (filtered test solution)[1]	2	ECHA

*There was increased turbidity of the test solutions with increasing concentrations; this indicates that effect concentrations exceeded the solubility of the test substance in the test medium.
**An average of 50% of the *Daphnia* were glued to oil drops at the surface or remained glued to the vessel walls.
[1]NOEC = 100 mg/L.

It should be noted that the water solubility of fatty acid ester (CAS No. 135800-37-2) is <0.05 mg/L (ECHA).

Chronic Studies

A 21-day *Daphnia* reproduction test was conducted on fatty acid ester (CAS No. 135800-37-2). The test substance was stirred for 16 hours to 7 days; after a settling period of 2 hours, the solution was filtered through a glass fiber filter (activated with 1 mL NaOH and washed with deionised water). There was 10% mortality at 100 mg/L, but no mortality in control and at 1 mg/L. For reproduction, the EC_{50} and NOEC were >100 and >1 mg/L, respectively (ECHA) [Kl. score = 1].

C. Terrestrial Toxicity

The 14-day LC_{50} of isopropyl myristate (CAS No. 110-27-0), a surrogate for fatty acid ester (CAS No. 135800-37-2), to earthworms was >20,000 mg/kg soil dry weight (ECHA). [Kl. score = 2]

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Fatty acid ester (CAS No. 135800-37-2) is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on the estimated BCF values, fatty acid ester (CAS No. 135800-37-2) does not meet the screening criteria for bioaccumulation.

The NOEC values from chronic aquatic toxicity studies on fatty acid ester (CAS No. 135800-37-2) are greater than its water solubility. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that fatty acid ester (CAS No. 135800-37-2) is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for fatty acid ester.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Fatty Acid Ester	135800-37-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	bioconcentration factor bioaccumulation factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EL	Effective loading
EU	European Union
hPa	hectopascal

IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN	USEPA organic carbon partition coefficient estimation model
KOWWIN	USEPA program to estimate the organic carbon-normalised sorption coefficient for soil and sediment
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mL	millilitre
mPa s	millipascal second
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction

FATTY ACID ESTER (CAS NO. 10024-47-2)

This dossier on fatty acid ester (CAS No. 10024-47-2) presents the most critical studies pertinent to the risk assessment of fatty acid ester (CAS No. 10024-47-2) in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Fatty acid ester is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Fatty acid ester (CAS No. 10024-47-2) is expected to be readily biodegradable. It is expected to have a low potential for bioaccumulation. It is highly insoluble in water and has high adsorption potential; thus, sediment and soil are expected to be the main targets for environmental distribution. Fatty acid ester (CAS No. 10024-47-2) is of low acute concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Fatty Acid Ester (CAS No. 10024-47-2)

CAS RN: 10024-47-2

Molecular formula: $C_{22}H_{42}O$

Molecular weight: 338.58 g/mol

Synonyms: Isobutyl oleate; 2-methylpropyl (Z)-octadec-9-enoate; 9-octadecenoic acid (9Z)-, 2-methylpropyl ester; oleic acid isobutyl ether; 2-methylpropyl (9Z)-octadec-9-enoate

3 PHYSICO-CHEMICAL PROPERTIES

No information is available on fatty acid ester (CAS No. 10024-47-2). Table 1 presents the physico-chemical properties of a structurally similar compound, isopropyl oleate (CAS No. 112-11-8).

Table 1 Overview of the Physico-chemical Properties of Isopropyl Oleate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	2	ECHA
Melting Point	-20°C (measured) @ 101.3 kPa	2	ECHA
Boiling Point	230°C @ 2.66 kPa (measured)	2	ECHA

Property	Value	Klimisch score	Reference
Density	870 kg/m^3 @ 20°C (measured)	2	ECHA
Vapour Pressure	0 Pa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	5.79 @ 20°C (measured)	2	ECHA
Water Solubility	<0.00015 g/L @ 20°C (measured)	2	ECHA
Dissociation Constant (pKa)	No dissociation	-	ECHA
Viscosity	4.6 mPa.s @ 40°C (measured)	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for fatty acid ester.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Fatty acid ester (CAS No. 10024-47-2) is expected to be readily biodegradable. It is expected to have a low potential for bioaccumulation. It is highly insoluble in water and has high adsorption potential; thus, sediment and soil are expected to be the main targets for environmental distribution.

B. Biodegradation

In an OECD 301B test, degradation of isopropyl oleate was >67.9% within the 10-day window; degradation was 98.2% after 28 days. These data indicate that isopropyl oleate is readily biodegradable (ECHA). [Kl. score = 1] If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for fatty acid ester (CAS No. 10024-47-2). Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 1,175,000 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 241,700 L/kg. When released to the environment, based on insolubility in water of structurally similar isopropyl oleate along with these estimated K_{oc} values, fatty acid esters (CAS No. 10024-47-2) are likely to partition to soil and sediment and be immobile.

D. Bioaccumulation

No experimental studies are available on fatty acid ester (CAS No. 10024-47-2). Using the BCFBAF module in EPISuite™ (USEPA, 2017), the estimated BCF for isobutyl oleate is 220.8 L/kg based on a regression based estimate.

Bioaccumulation would also not be expected due to the rapid hydrolysis of fatty acid ester (CAS No. 10024-47-2) to the alcohol and fatty acid by the enzyme carboxylesterase. Both the alcohol and fatty acid can be extensively metabolised and excreted.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Fatty acid ester (CAS No. 10024-47-2) is of low acute concern to aquatic organisms, at least in the range of its water solubility.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 lists the results of acute aquatic toxicity studies on fatty acid ester (CAS No. 10024-47-2) and surrogates.

Table 3 Acute Aquatic Toxicity Studies on fatty acid ester (CAS No. 10024-47-2) and Surrogates.

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Cyprinus carpio	96-hour LC_{50}	>100*	2	ECHA
Daphnia magna	48-hour EC_{50}	>3,000**	2	ECHA
Scenedesmus subspicatus	72-hour EC_{50} 72-hour EL_{50} NOEC	<100 >100 (WAF) 100 (WAF)	2	ECHA

*Test substance is isopropyl oleate; droplets were seen at the surface of the test medium.
**Test substance is isopropyl palmitate (CAS No. 142-91-6). The ECHA database states: “Only the dissolved material was applied to avoid physical influence of the test substance. Analytical retrieval of solved substance was below 0.1%.”

Chronic Studies

Since no studies are available for the long-term aquatic invertebrate toxicity of fatty acid ester (CAS No. 10024-47-2) or its surrogate isopropyl oleate (CAS No. 112-11-8), the assessment was based on a study conducted with the structurally most similar substance, for which data is available (Fatty acids, C16-18 and C18 unsaturated isobutyl esters [CAS No. 84988-79-4]) as part of a read-across approach. A 21-day *Daphnia* reproduction study was conducted on the surrogate. The EL_{50} and a NOEL were >100 mg/L WAF (ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

The 14-day LC_{50} of isopropyl myristate (CAS No. 110-27-0) to earthworms was >20,000 mg/kg soil dry weight (ECHA). [Kl. score = 2]

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Fatty acid ester (CAS No. 10024-47-2) is expected to be readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on the estimated BCF of 220.8 L/kg, fatty acid ester (CAS No. 10024-47-2) does not meet the screening criteria for bioaccumulation.

There were no acute or chronic effects seen in the aquatic toxicity studies at the level of the water solubility of fatty acid ester (CAS No. 10024-47-2) or its surrogates. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that fatty acid ester (CAS No. 10024-47-2) is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for the fatty acid ester.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
fatty acid ester	10024-47-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	bioconcentration factor bioaccumulation factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system

KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mm^2/s	square millimetres per second
NOEC	no observed effective concentration
NOEL	no observed effect level
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
WAF	water accommodated fraction

FOOD RED 10

This dossier on Food Red 10 presents the most critical studies pertinent to the risk assessment of Food Red 10 in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Food Red 10 is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Food Red 10 will strongly adsorb to soil or sediment and have a low potential for mobility in soil. However, it is inherently biodegradable, not persistent, and not expected to bioaccumulate. No aquatic toxicity studies are available on Food Red 10. Based on QSAR modelling, it is expected to be of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium 5-acetamido-4-hydroxy-3-(phenyldiazenyl)naphthalene-2,7-disulfonate

CAS RN: 3734-67-6

Molecular formula: $C_{18}H_{13}N_3Na_2O_8S_2$

Molecular weight: 509.42 g/mol

Synonyms: Disodium 5-acetamido-4-hydroxy-3-(phenyldiazenyl)naphthalene-2,7-disulfonate; Disodium 5-acetamido-4-hydroxy-3-(phenyazol)naphthalene-2,7-disulfonate; Acid red 1; Food Red 10; Red 2G; potacyl carmine; amidonaphthol red; disodium (3E)-5-acetamido-4-oxo-3-(2-phenylhydrazinylidene)naphthalene-2,7-disulfonate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Food Red 10

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Red powder or granules	2	ECHA
Melting Point	349.84°C (estimated*)	2	USEPA, 2017
Boiling Point	942.84°C (estimated*)	2	USEPA, 2017
Density	1774 kg/m^3@ 20°C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	-	-	-
Partition Coefficient (log K_{ow})	-2.392 @ 20°C	2	ECHA
Water Solubility	132 g/L @ 20°C	1	ECHA

*Estimated using QSAR models. Pressure not provided

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for Food Red 10.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Food Red 10 will strongly adsorb to soil or sediment and have a low potential for mobility in soil. However, it is inherently biodegradable and not persistent. It is also not expected to bioaccumulate.

B. Biodegradation

Food Red 10 is inherently biodegradable. In the key study, Jahir Alam Khan (2011) studied the biodegradation of Azo Dye by Moderately Halotolerant Bacillus megaterium in water. Percentage dye degradation by the isolated Bacillus megaterium was found to be 64.89% in 20 days (ECHA). [Kl. Score = 2]. If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017). EPISuite™ estimated a half-life in soil of 120 days @ 25 °C. Therefore, Food Red 10 is estimated not be persistent in the soil environment as well (ECHA).

C. Environmental Distribution

No experimental data are available for Food Red 10. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from the molecular connectivity index (MCI) is 779.4 L/kg. Based on this estimated K_{oc} value, this substance will strongly sorb to soil or sediment and have low to moderate mobility.

D. Bioaccumulation

No bioconcentration studies have been conducted on Food Red 10. The experimental log K_{ow} of Food Red 10 is -4.79 (ECHA). Using the BCFBAF model in EPISuite™ (USEPA, 2017), the estimated BCF of Food Red 10 is 3.162 L/kg. Thus, Food Red 10 is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No aquatic toxicity studies are available on Food Red 10. Based on QSAR modelling, it is expected to be of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

No experimental studies are available. Using ECOSAR in EPISuite™ (USEPA, 2017), the estimated acute toxicity values are as follows: 96-hour LC_{50} in fish is 1,074 mg/L; the 48-hour EC_{50} in *Daphnids* is 12,403 mg/L; and the 96-hour EC_{50} in algae is 197 mg/L. All of these values are at least 10-fold higher than the estimated water solubility of Food Red 10 of 3.957 mg/L. ECOSAR instructs that typically no effects at saturation are reported if the effect level exceeds the water solubility by 10x.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Food Red 10 is inherently biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -4.7 and a calculated BCF of 3.162 L/kg, Food Red 10 does not meet the screening criteria for bioaccumulation.

There are no experimental data on the aquatic toxicity of Food Red 10. The estimated acute EC_{50} values for Food Red 10 in fish, invertebrates, and algae from QSAR modelling are >1 mg/L. Thus, Food Red 10 does not meet the screening criteria for toxicity.

The overall conclusion is that Food Red 10 is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for Food Red 10.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Food Red 10	3734-67-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	USEPA modelling program to estimate bioconcentration factor bioaccumulation factors
BIOWIN	USEPA modelling program to estimate biological degradation
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
ECOSAR	USEPA modelling program to estimate aquatic toxicity
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogrrams per cubic metre
Kl	Klimisch scoring system

KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

FORMIC ACID

This dossier on formic acid presents the most critical studies pertinent to the risk assessment of the substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Formic acid is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Formic acid is the simplest carboxylic acid. It is an important intermediate in chemical syntheses and occurs naturally, most notably in some ants. The substance has low aquatic toxicity, readily biodegrades and is not expected to bioaccumulate.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Methanoic acid

CAS RN: 64-18-6

Molecular formula: CH_2O_2

Molecular weight: 46.025 g/mol

Synonyms: Carbonous acid; Formylic acid; Hydrogen carboxylic acid; Hydroxy(oxo)methane; Metacarbonoic acid; Oxocarbinic acid; Oxomethanol

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Formic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	clear and colourless liquid	1	ECHA
Melting Point	8 °C (Pressure not provided)	1	ECHA
Boiling Point	100.23 °C @ 101.3 kPa	1	ECHA
Density	1220 kg/m^3 @ 20 °C	1	ECHA
Vapor Pressure	4271 Pa @ 20 °C	1	ECHA
Partition Coefficient (log K_{ow})	-2.1 at 23 °C and pH 7	1	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	1,000 g/L @ 25 °C	-	PubChem
Dissociation Constant (pKa)	3.7 @ 20 °C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for formic acid.

NICNAS has assessed formic acid in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Formic acid is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment.

B. Partitioning

The pKa of formic acid is 3.7, indicating that this substance will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts (PubChem).

Volatilisation of formic acid from water and moist soil surfaces is expected to be an important fate process given a Henry's Law constant of 0.017 Pa-m^3/mole (ECHA). Formic acid is expected to volatilise from dry soil surfaces based upon its vapour pressure.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=64-18-6%2C+

Hydrolysis is not expected to be an important environmental fate process since this substance lacks functional groups that hydrolyse under environmental conditions(PubChem).

C. Biodegradation

Formic acid and the formate ion were readily biodegradable in OECD 301 D tests. In the two tests, biodegradation rates of 82% and 92 % related to the biological oxygen demand were estimated. (ECHA) [Kl. score = 1 and Kl. Score =2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

The log K_{oc} of the non-dissociated species of formic acid was measured to be < 1.25 in a GLP test according to OECD guideline 121. As this value refers to the uncharged molecule, which will only be present under highly acidic conditions, the K_{oc} and log K_{oc} of the dissociated, charged form at realistic environmental pH values was calculated by using the pKa (= 3.70) and the log P_{ow} of the uncharged molecule (= -0.46) for a corrected log K_{oc} according to Franco et al. (2008). For the formate ion which will be present at environmental relevant pH values, slightly higher adsorption rates were estimated (K_{oc} = 31, log K_{oc} = 1.49) (BASF SE, 2009) (ECHA) [Kl. Score = 2].

Based on these values, formic acid has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil. Likewise, if released to water, formic acid is also not expected to adsorb to suspended solids or sediments.

E. Bioaccumulation

No bioconcentration studies have been conducted on formic acid. Formic acid is not expected to bioaccumulate based on the experimental log K_{ow} of -2.1 (ECHA) [Kl. Score = 1].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Formic acid is of low toxicity to aquatic organisms on an acute and chronic basis.

A. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on formic acid.

Table 3 Acute Aquatic Toxicity Studies on formic acid

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachydanio rerio	96-hr LC50	130*	1	ECHA
Daphnia magna	48-hr EC50	365*	1	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pseudokirchneriella subcapitata	72-hr EC50	1,240**	1	ECHA

*Potassium formate
**Ammonium formate

Chronic Studies

In a 21-day *Daphnia* reproduction study, the measured NOEC for formic acid was 100 mg/L (ECHA). [Kl. score = 1]

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Formic acid is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The experimental log K_{ow} for formic acid is -2.1. Thus,formic acid does not meet the criteria for bioaccumulation.

The NOEC from the chronic aquatic toxicity study on formic acid is >0.1 mg/L. The acute EC_{50} values from the acute aquatic toxicity studies on formic acid are >1 mg/L. Thus, formic acid does not meet the criteria for toxicity.

The overall conclusion is that formic acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for formic acid.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Formic acid	64-18-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

DoEE. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

GELATINS

This dossier on gelatins presents the most critical studies pertinent to the risk assessment of gelatins in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Gelatins are classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Gelatin is a biopolymer derived from collagen, a naturally occurring protein. In the coal seam gas industry, gelatin is used in hydraulic fracturing as an oxygen scavenger/corrosion inhibitor (Government of Western Australia - Department of Mines and Petroleum 2015).

Gelatins are not bioaccumulative nor toxic. The natural decay and/or breakdown of this substance is unlikely to cause harm in the environment or to human health.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Gelatins

CAS RN: 9000-70-8

Molecular formula: Not applicable as substance is a UVCB whose specific chemical composition is dependent on formulation processes.

Molecular weight: Depending on the specific commercial use, the molecular weight can range from 72 to 132 kDaltons (i.e., 72,000 to 132,000 g/mol (Farrugia et. al., 1998)).

Synonyms: None identified.

3 PHYSICAL AND CHEMICAL PROPERTIES

Gelatin is a white to yellow, translucent powder. It is hydrolysed and partially degraded collagen obtained by acid, alkaline, or enzymatic hydrolysis. It is a polypeptide and depending on the source of collagen and the method of its manufacturing process of recovery from collagen, gelatin contains an average of the following amino acids: glycine 21%, proline 12%, hypoproline 12%, glutamic acid 10%, alanine 9%, arginine 8%, aspartic acid 6%, lysine 4%, serine 4%, leucine 3%, valine 2, phenylalanine 2%, threonine 2%, isoleucine 1%, hydroxylysine 1%, histidine <1% and tyrosine <0.5% (Gorgieva and Kokol 2011).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for gelatins.

NICNAS has assessed gelatin in an IMAP Tier 1 assessment and it was concluded that it poses no unreasonable risk to the environment[1]. In addition, based on an assessment of human health and environmental hazards, NICNAS also identified gelatin as a chemical of low concern to the environment (NICNAS, 2017 and DoEE, 2017). Chemicals of low concern are unlikely to have adverse environmental effects or be a concern to human health if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE PROPERTIES

A. Summary

Gelatins are readily biodegradable; they are not expected to bioaccumulate or adsorb to soil.

B. Biodegradation

As a natural polymer, gelatin is expected to be readily biodegradable by most proteases when environmental conditions are adequate. While high molecular weight polymer degradation rates are generally thought to be low, the biopolymeric nature of gelatin in a variety of cross-linked forms appears to result in rapid biodegradation (e.g., 3-10 days) in the environment (Patel et. al. 2000).

Gelatin as a rapidly biodegradable protein is a rich source of amino acids and other nutrients such as nitrogen and carbon for bacteria and fungi. The increased bioavailability of nutrients could lead to a significant increase in biological oxygen demand (BOD) as a result of degradation of gelatin and the stimulated growth of microorganisms. High BOD will deplete local dissolved oxygen concentrations when gelatin or its breakdown products are released into the aquatic environment in sufficient quantities relative to the volume of the receiving water body. This depletion of oxygen has the potential to place significant stress on some organisms within the aquatic environment (DoEE, 2017).

C. Environmental Distribution

Given the hydrophilic nature of gelatin it is unlikely that this biopolymer would adsorb to the soil or sediment.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9000-70-8%2C+

D. Bioaccumulation

The potential for bioaccumulation is low. Based on the biological properties and the environmental fate of gelatin, especially the rapid biodegradation, prolonged exposure of aquatic organisms to the biopolymer will be highly unlikely (DoEE, 2017).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

There are no aquatic toxicity studies on gelatin. However, it is expected to have low concern for aquatic toxicity since any gelatin released into aquatic ecosystems will be rapidly degraded by microorganisms through enzymatic digestion to the individual amino acids or short peptides. If sufficient quantities of gelatin were abruptly released into a water body, this could cause temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations (DoEE, 2017).

B. Aquatic Toxicity

No aquatic toxicity data were available.

C. Terrestrial Toxicity

No relevant studies were available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Gelatins are readily biodegradable; thus it does not meet the screening criteria for persistence.

The rapid degradation and expected lability to enzymatic degradation suggests gelatins will not meet the screening criteria for bioaccumulation.

There are no aquatic toxicity studies on gelatins. It is expected to have low concern for aquatic toxicity because of its bio-composition (e.g., various amino acids and crosslinked substituents) and rapid degradation rates in the environment. Thus, gelatin does not meet the screening criteria for toxicity.

The overall conclusion is that gelatin is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for gelatins.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Gelatins	9000-70-8	Not a PBT	No	No	No	No	No	No	No data	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Acronyms and Glossary

AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
COD	chemical oxygen demand
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
ECHA	European Chemicals Agency
EU	European Union
g/kg	grams per kilogram
g/mole	grams per mole
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

GLASS, OXIDE

This dossier on glass, oxide does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies pertinent to the risk assessment of glass, oxide in its use in coal seam gas extraction activities. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Glass oxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

This category encompasses the various chemical substances manufactured in the production of inorganic glasses. For purposes of this category, 'glass' is defined as an amorphous, inorganic, transparent, translucent or opaque material traditionally formed by fusion of sources of silica with a flux, such as an alkali-metal carbonate, boron oxide, etc. and a stabilizer, into a mass which is cooled to a rigid condition without crystallization in the case of transparent or liquid-phase separated glass or with controlled crystallization in the case of glass-ceramics. The category consists of the various chemical substances, other than by-products or impurities, which are formed during the production of various glasses and concurrently incorporated into a glass mixture (ECHA).

Glass, oxide is inorganic, chemically inert and highly insoluble in water. Biodegradation is not applicable to this inorganic substance and bioaccumulation is not expected. This substance is of low toxicity concern to aquatic and terrestrial receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): silicon(4+) dialuminium(3+) diboron(3+) octaoxidandiide

CAS RN: 65997-17-3

Molecular formula: Not applicable as substance is a UVCB

Molecular weight: variable (UVCB)

Synonyms: glass oxide, chemicals; calcium sodium phosphate; rhenanite; fiberglass

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Glass, Oxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White solid fibre, odorless	2	ECHA
Melting Point	~800 °C @ 101.3 kPa	3	ECHA
Boiling Point	Not applicable	-	ECHA
Density	2600 kg/m^3 @ 20 °C	3	ECHA
Water Solubility	highly insoluble in water	-	ECHA
Dissociation Constant (pKa)	Not applicable	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for glass, oxide.

NICNAS has assessed glass, oxide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1]. It is an inorganic substance with low toxicity and/or low bioavailability. It is a low concern to the environment.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Glass, oxide is an inorganic, chemically inert substance. It is highly insoluble in water and not subject to hydrolysis. Biodegradation is not applicable to this inorganic substance. Due to its physico-chemical properties (inorganic and highly insoluble in water), glass, oxide has low potential for adsorption to soil and sediment and bioaccumulation is not expected (ECHA).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=65997-17-3

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Glass, oxide is of low toxicity concern to aquatic or terrestrial receptors.

B. Aquatic Toxicity

Acute Studies

Table 3: Acute Aquatic Toxicity Studies on Glass, oxide*

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio (Zebra fish)	96-h LC_{50}	>1000	1	ECHA
Daphnia magna	72-h EC_{50}	> 1000	1	ECHA
Raphidocelis subcapitata (previous name *Pseudokirchneriella subcapitata)*	72-h LC_{50}	>1000	1	ECHA

*MMVF (man-made vireous (silicate) fibre

Chronic Studies

There are no chronic studies for fish or invertebrates. Due to the known inherent physico-chemical properties and the absence of acute toxic effects, there is no indication for harmful long-term effects arising from exposure to glass, oxide.

The72-hour NOEC for *Raphidocelis subcapitata* is ≥ 1000 mg/L for MMVF (ECHA) [KI Score 1].

C. Terrestrial Toxicity

There were no terrestrial studies conducted using glass, oxide or MMVF. The substance is considered harmless to the environment and environmental organisms (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Biodegradation is not applicable to glass, oxide, an inorganic substance. For the purposes of this PBT assessment, the persistent criteria is not considered applicable to glass, oxide.

Due to the fact that this fibre is an inorganic inert substance that is not bioavailable, bioaccumulation is not expected. Thus, glass, oxide does not meet the criteria for bioaccumulation.

The lowest chronic toxicity value for glass oxide is >0.1 mg/L. The acute E(L)C_{50} values for glass, oxide is >1 mg/L. Thus, it does not meet the criteria for toxicity.

The overall conclusion is that glass, oxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for glass, oxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Glass, oxide	65997-17-3	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia. Available: http://www.nepc.gov.au/resource/chemical-risk-assessment-guidance-manuals

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/kg	grams per kilogram
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre

MMVF	man-made vitreous (silicate) fibres
NOEC	No observed effect concentration
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	unknown or variable composition, complex reaction products or of biological materials

GLYCERINE
[GLYCEROL]

This dossier on glycerine presents the most critical studies pertinent to the risk assessment of glycerine in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on glycerol (OECD, 2002), and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Glycerine is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Glycerine is readily biodegradable. It is not expected to bioaccumulate. Based on the estimated K_{oc} value, glycerine is expected to be highly mobile in sediment and soil. Glycerine is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Glycerol

CAS RN: 56-81-5

Molecular formula: $C_3H_8O_3$

Molecular weight: 92.09 g/mol

Synonyms: Glycerine; glycerin; glycerol; glycyl alcohol; 1,2,3-propanetriol; trihydroxypropane

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Glycerine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear, water-white, viscous, sweet-tasting hygroscopic liquid.	2	ECHA
Melting Point	18.17°C @ 101.3 kPa	2	ECHA
Boiling Point	290°C @ 101.3 kPa	2	ECHA
Density	1261 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	0.01 Pa @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-1.75 @ 25°C (measured)	2	ECHA
Water Solubility	1000 g/L @ 25°C (completely miscible)	2	ECHA
Viscosity	1412 mPa.s at 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for glycerine.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Glycerine is readily biodegradable. It is not expected to bioaccumulate. Based on the estimated K_{oc} value, glycerine is expected to be highly mobile in sediment and soil.

B. Biodegradation

Glycerine was readily biodegradable in an OECD 301D test. Degradation was 57% after 5 days, 84% after 15 days, and 92% after 30 days (OECD, 2002) [Kl. score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for glycerine. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 0.1345 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 1 L/kg.

Based upon these K_{oc} values, if released to soil, glycerine is expected to have low potential for adsorption and a high potential for mobility. If released to water, based on its K_{oc} and high water solubility, glycerine is likely to remain in water and not adsorb to sediment.

D. Bioaccumulation

No bioconcentration studies have been conducted on glycerine. Glycerine is not expected to bioaccumulate based on the experimental log K_{ow} of -1.75 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Glycerine is of low toxicity concern to environmental receptors.

Glycerine is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on glycerine.

Table 3 Acute Aquatic Toxicity Studies on Glycerine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	54,000	2	ECHA
Sheepshead minnow	96-hour LC_{50}	>11,000	2	ECHA
Daphna magna	24-hour EC_{50}	>10,000	2	ECHA
Scenedesmus quadricauda	8-day EC_{50}	>10,000	2	Bringmann and Kuehn, 1980; OECD, 2002

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Glycerine is readily biodegradable and thus does not meet the screening criteria for persistence.

No bioconcentration studies are available for glycerine. The measured log K_{ow} for glycerine is -1.75; thus glycerine does not meet the screening criteria for bioaccumulation.

The acute EC_{50} values for glycerine in fish, invertebrates, and algae are >1 mg/L. Thus glycerine does not meet the screening criteria for toxicity.

The overall conclusion is that glycerine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for glycerine.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Glycerine	56-81-5	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Bringmann, G., and Kuehn, R. (1980). Comparison of the toxicity thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water. Res. 14: 231-241.

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Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration

ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mm	millimetre
OECD	Organisation for Economic Co-operation and Development
Pa s	pascal second
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

GLYOXAL

This dossier on glyoxal presents the most critical studies pertinent to the risk assessment of glyoxal in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on glyoxal (OECD, 2005) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Glyoxal is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Glyoxal is a non-volatile liquid at room temperature and is commonly supplied commercially as a 40% aqueous solution. Glyoxal is readily biodegradable and is not expected to bioaccumulate. Glyoxal exhibits a low concern for toxicity to aquatic organisms, as well as to terrestrial invertebrates and plants.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Oxalaldehyde

CAS RN: 107-22-2

Molecular formula: $C_2H_2O_2$

Molecular weight: 58.04 g/mol

Synonyms: 1,2-ethanedial, biforrmal, biformyl, ethandedial (9CI), ethandione, glyoxal, glyoxal aldehyde, oxal,

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Glyoxal

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	Clear, slightly viscous liquid	1	ECHA
Melting Point*	-25°C @ 101.3 kPa	1	ECHA
Boiling Point*	103.6°C @ 101.3 kPa	1	ECHA
Density*	1270 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure*	2020 Pa @ 20°C	1	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log P_{ow})*	-1.15 @ 23°C (pH 7) -1 @ 23°C (pH 5) -1.62 @ 23°C (pH 9)	1	ECHA
Water Solubility*	Miscible (20°C, pH 5-9)	1	ECHA
Viscosity	8.37 mPa.s (dynamic) @ 20°C	1	ECHA

*40% glyoxal in water

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for glyoxal.

Based on an assessment of environmental hazards, NICNAS identified glyoxal as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Glyoxal is readily biodegradable. Glyoxal is mobile in soil and it has a low potential for accumulation in soil. It is also not expected to bioaccumulate based on the octanol-water partition coefficient.

B. Abiotic Degradation

Hydrolysis

Anhydrous glyoxal immediately reacts with water to form ethane bis-gemdiol, which is stable in water. Polymerisation to acetals-semiacetals is possible, depending on concentration and pH (OECD, 2005).

C. Biodegradation

The results from biodegradation studies are shown in Table 3. Glyoxal is readily biodegradable.

Table 3 Biodegradation Studies on Glyoxal

Test Method	Results	Klimisch score	Reference
OECD 301A	>90% after 19 days	1	ECHA
OECD 301C	65% (BOD/ThOD), 98% (TOC removal) after 14 days	2	ECHA
OECD 301D	90% after 28 days	2	ECHA

D. Environmental Distribution

Adsorption/desorption

An experimental K_{oc} of a 40% aqueous solution of glyoxal was determined to be 2.1 L/kg from an OECD TG 121 test (OECD, 2005; ECHA). [Kl. score = 1]

Distribution Modelling

According to a MacKay Level I fugacity model, all (100%) of the released glyoxal would be in the water compartment (OECD, 2005). A MacKay Level III fugacity model gave the following results: air (0.1%), water (45.6%), sediment (0.1%) and soil (54.2%). If released to air, glyoxal would rapidly partition to soil and water; if released to soil and water, glyoxal would mostly remain in those compartments and degradation would prevent partitioning from one compartment to the other (OECD, 2005).

E. Bioaccumulation

No experimental studies on glyoxal were identified. The octanol-water partition coefficient is -1.15 at pH 7 (ECHA), indicating a low potential for bioaccumulation.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Glyoxal exhibits a low concern for toxicity to aquatic organisms, as well as to terrestrial invertebrates and plants.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on glyoxal.

Table 4 Acute Aquatic Toxicity Studies on Glyoxal

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Golden orfe	96-hour LC_{50}	186 - 272	2	ECHA
Common carp	96-hour LC_{50}	>200	2	ECHA
Pimephales promelas	96-hour LC_{50}	215	2	ECHA
Daphnia magna	48-hour EC_{50}	101	2	ECHA
Scenedesmus subspicatus	72-hour EC_{50} 72-hour NOEC	>200 >100	2	ECHA
Scenedesmus subspicatus	72-hour EC_{50} 72-hour NOEC	>100 3.13	1	ECHA

Chronic Studies

The chronic aquatic toxicity studies conducted on glyoxal are listed in Table 5.

Table 5 Chronic Aquatic Toxicity Studies on Glyoxal

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fathead minnow	34-day NOEC	112	1	ECHA
Daphnia magna	21-day NOEC	3.19	1	ECHA

C. Terrestrial Toxicity

Table 6 lists the results of toxicity studies conducted on glyoxal with earthworms, soil microorganisms and birds.

Table 6 Terrestrial Toxicity Studies on Glyoxal

Test Species (method)	Endpoint	Results (mg/L)	Klimisch score	Reference
Earthworm Eisenia fetida (OECD 207)	14-day LC_{50}	>398	1	ECHA
Soil microorganisms (OECD 216)*	28-day EC_{50} 28-day EC_{10}	>400 >400	1	ECHA
Soil microorganisms (OECD 217)*	28-day EC_{50} 28-day EC_{10}	>400 240	1	ECHA

*organic carbon content of soil = 1.34% dry weight

Glyoxal has also been evaluated in a terrestrial plants test: seedling emergence and seedling growth test (OECD TG 208). The test material contained 40% glyoxal. The results are as follows (expressed as active ingredient):

Avena sativa (oats): 19-day EC_{50} value is >400 mg/kg soil dry weight based on emergence rate, fresh matter, dry matter and shoot length. The NOECs were >400 mg/kg soil dry weight on tested parameters.

Brassica napus (rapeseed): 19-day EC_{50} is >400 mg/kg soil dry weight based on emergence rate, fresh matter, dry matter and shoot length. The NOEC was >400 mg/kg soil dry weight for seedling emergence and 503 mg/kg soil dry weight for dry matter, fresh matter and shoot length.

Vicia sativa (vetch): 19-day EC_{50} is >400 mg/kg soil dry weight based on emergence rate, fresh matter, dry matter and shoot length. The NOEC was >400 mg/kg soil dry weight for seedling emergence and 203 mg/kg soil dry weight for fresh matter and dry matter (ECHA). [Kl. score = 1]

7 CATEGORISATION AND OTHER CHARACTIERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Glyoxal is readily biodegradable; Therefore, it does not meet the screening criteria for persistence.

The estimated log K_{ow} value for glyoxal is -1.15. Therefore, glyoxal does not meet the screening criteria for bioaccumulation.

Chronic NOECs for fish, invertebrates and algae are available for glyoxal and the NOEC values are >0.01 mg/L. Therefore, glyoxal does not meet the screening criteria for toxicity.

The overall conclusion is that glyoxal is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for glyoxal.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Glyoxal	107-22-2	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA) (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	Biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre

Kl	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa m^3/mol	pascal meter cubed per gram molecular weight
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
ThOD	Theoretical oxygen demand
TOC	Total organic carbon

GRAPHITE

This dossier on graphite presents the most critical studies pertinent to the risk assessment of graphite in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Graphite is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Graphite is a naturally-occurring form of crystalline carbon. It is a native element mineral found in metamorphic and igneous rocks. It is extremely soft, cleaves with very light pressure, and has a very low specific gravity. In contrast, it is extremely resistant to heat and nearly inert in contact with almost any other material.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Carbon

CAS RN: 7782-42-5

Molecular formula: [C]

Molecular weight: 12.011 g/mol

Synonyms: Carbon powder, carbon black

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Graphite

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Odourless black solid powder	-	ECHA
Melting Point	600°C @ 101.3 kPa	-	ECHA
Boiling Point	Study not necessary according to Annex VII column II REACH-Regulation for substances with a melting point higher than 300°C.	-	ECHA
Density	2214 kg/m^3 @ 25°C	-	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	Study not necessary according to Annex VII column II REACH-Regulation for substances with a melting point higher than 300°C.	1	ECHA
Partition Coefficient (log K_{ow})	Study not necessary according to Annex VII column II REACH-Regulation for inorganic substances.	1	ECHA
Water Solubility	0 g /L @ 25°C (insoluble)	1	ECHA
Viscosity	The study is technically not feasible because the OECD test guideline No. 114 is applicable to liquids only.	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for graphite.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Graphite is an inorganic substance that is not subject to biodegradation, is not expected to bioaccumulate;and, being chemically inert and insoluble, adsorption is not relevant .

B. Biodegradation

Graphite is an inorganic substance. According to Annex VII of the REACH regulations, biodegradation testing for inorganic chemicals is not required.

C. Environmental Distribution

No value for the adsorption /desorption is given due to the technical infeasibility to detect the substance graphite in the solvents used for the test (ECHA).

D. Bioaccumulation

A bioaccumulation study is technically not feasible according to REACH Annex XI, point 2. Based on its physicochemical properties it can safely be concluded that graphite is devoid of any bioaccumulation potential.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Graphite is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

The short-term fish toxicity was determined to be > 100 mg/L for the LC_{50} and > 100 mg/L for the NOEC, following Testing guidelines OECD 201 as well as EU C1(ECHA) [Kl Score = 2].

The short-term toxicity for aquatic invertebrates (*daphnids*) was determined to be > 100 mg/L for the EC_{50} and > 100 mg/L for the NOEC, following Testing guidelines OECD 202 as well EU C.2 (ECHA) [Kl Score = 2].

Based in the result obtained by a valid GLP-OECD 201 study in algae with graphite as test item, no toxic effects were found up to the highest tested concentration of 100 mg/L(ECHA) [Kl Score = 2].

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Graphite is an inorganic mineral. Thus, biodegradation is not applicable to this substance. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to graphite.

OECD test guideline 305 on bioaccumulation in fish is applicable to chemical substances for which it is possible to generate stable solutions in water. Graphite, however, is completely insoluble in water.

In view of its insolubility, there is no bioaccumulation potential of graphite under realistic natural conditions.

The NOECs from the acute aquatic toxicity studies on graphite are greater than 1 mg/L. Thus graphite, does not meet the criteria for toxicity.

Thus, graphite is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for graphite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Graphite	7782-42-5	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
GLP	Good Laboratory Procedures
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

GUAR GUM

This dossier on guar gum presents the most critical studies pertinent to the risk assessment of guar gum in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the chemistry database PubChem. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion –Guar Gum was assessed as a tier 1 chemical based on acute toxicity studies. It has low acute toxicity concern for fish, but exhibits medium or possibly high acute toxicity to invertebrates (*Daphnia*). However, guar gum is unlikely to have long-term environmental effects because the carbohydrate chemical nature of the substance is expected to render it readily biodegradable. Therefore, guar gum is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Guar gum (CAS No. 9000-30-0) is a resinous material derived from milled endosperm from guar beans of the legume Cyamopsis tetragonolobus. Structurally, it is a galactomannan (high molecular weight carbohydrate polymer) consisting of a main chain of D-mannose with a side chain of D-galactose at approximately every second mannose unit. It is expected to be readily biodegradable and not bioaccumulate. It has low acute toxicity concern for fish, but exhibits medium or possibly high acute toxicity to invertebrates (*Daphnia*).

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): disodium;[[[5-(6-aminopurin-9-yl)-3-hydroxyoxolan-2-yl]oxy-methoxyphosphoryl]oxy-oxidophosphoryl] hydrogen phosphate

CAS RN: 9000-30-0

Molecular weight: 535.15 gm/mol; 200,000 to 300,000 daltons (Glickman, 1969)

Molecular formula: $C_{10}H_{14}N_5Na_2O_{12}P_3$

Synonyms: GU-052, guar flour, guaran, gum guar, slocose

3 PHYSICO-CHEMICAL PROPERTIES

Available physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Guar Gum

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Off-white to yellowish-white powder	-	PubChem
Vapour Pressure	Negligible	-	PubChem

Property	Value	Klimisch score	Reference
Water Solubility	< 1 g/L @ 20 °C (insoluble)	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for guar gum.

NICNAS has assessed Guar Gum in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Guar gum is a carbohydrate polymer consisting of D-mannose and D-galactose sugars from the guar plant or cluster bean. As a high molecular weight polysaccharide polymer, guar gum is expected to have a negligible vapour pressure. If released to air, a negligible vapour pressure indicates guar gum will exist solely in the particulate phase in the atmosphere. Particulate-phase guar gum will be removed from the atmosphere by wet and dry deposition. If released to soil, guar gum is expected to have no mobility since it is a polymer that binds strongly with soil particles. Volatilisation from moist soil surfaces is not expected to be an important fate process based upon a negligible Henry's Law constant. Likewise, guar gum is not expected to volatilise from dry soil surfaces based upon its vapour pressure. If released into water, guar gum is expected to adsorb to suspended solids and sediment (PubChem). Half-life data was not available.

Guar gum is expected to readily undergo microbial biodegradation in the environment (on the bases that is polysaccharide and expected to be readily biodegradable), and the potential to bioaccumulate in organisms is considered to be low (DoEE, 2017 and US EPA, 2005).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9000-30-0%2C+

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Guar gum is a polysaccharide polymer. It has low acute toxicity concern for fish, but exhibits medium or possibly high acute toxicity to invertebrates (*Daphnia*).

B. Aquatic Toxicity

The 96-hour LC_{50} for *Oncorhynchus mykiss* is 218 mg/L (Biesinger *et al.*, 1976). [Kl. score = 2]

The 48-hour and 96-hour LC_{50} values for *Daphnia magna* are 42 mg/L and <6.2 mg/L, respectively (Biesinger *et al.*, 1976). [Kl. score = 2]

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Guar gum is a naturally occurring polysaccharide from the guar plant or cluster bean; it is expected to be readily biodegradable. Thus it is not expected to meet the screening criteria for persistence.

The molecular weight of guar gum ranges from 200,000 to 300,000 daltons and is water-soluble. Thus guar gum is not expected to meet the criteria for bioaccumulation.

The 96-hour LC_{50} value for *Daphnia* is <6.2 mg/L. Thus guar gum may potentially meet the screening criteria for toxicity.

Therefore, guar gum is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for guar gum.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Guar Gum	9000-30-0	Not a PBT	No	No	No	No	No	Potentially Yes	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Biesinger, K.E., Lemke, A.E., Smith, W.E., and Tyo, R.M. (1976). Comparative toxicity of polyelectrolytes to selected aquatic animals. J. Water Pollut. Control Fed. 48: 183-187; cited in U.S. EPA ECOTOX database.

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Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Glickman M. (1969). Gum technology in the Food Industry, pp. 590, Academic Press, New York; cited in Yoon et al. (1998).

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B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency

EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
LC	lethal concentration
mg/L	milligrams per litre
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

HEMICELLULASE ENZYMES

This dossier on hemicellulase enzyme presents the most critical studies pertinent to the risk assessment of hemicellulase enzyme in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Hemicellulase enzymes are classified as a **tier 1** chemical and require a hazard assessment only.

1 BACKGROUND

Hemicellulase enzymes are catalytic proteins or polypeptides that consist of amino acids coupled via peptide bonds. Hemicellulases are a group of enzymes that break down hemicellulose, which are polysaccharides that are present in cell walls of all terrestrial plants. These polysaccharides have a β-(1→4)-linked backbone and are composed of pentoses (xylose, arabinoses), hexoses (mannose, glucose, galactose), and sugar acids. No information was located on the physico-chemical properties, environmental fate, human health and ecological toxicity of hemicellulase enzymes. There are, however, data on cellulase enzymes (they cleave the ß-1,4-glycosidic bonds in cellulose), which are expected to have similar properties to the hemicellulase enzymes. Cellulase enzyme is readily biodegradable, and is expected not to bioaccumulate or adsorb to soil. Cellulase enzymes have a moderate acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Hemicellulase

CAS RN: 9025-56-3

Molecular weight: 20,000 to 80,000 g/mol (based on cellulase enzyme)

Molecular formula: Not applicable

Synonyms: Hemicellulase

3 PHYSICO-CHEMICAL PROPERTIES

No information is available on the hemicellulase enzymes. Key physical and chemical properties for cellulase (CAS No. 9012-54-8) are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Cellulase

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	As pure enzyme, white crystals or powder	-	HERA, 2005
Melting Point	Not feasible	-	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	Not feasible	-	ECHA
Density	>1330 - <1420 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	0.00344 Pa @ 25°C (mean value)	1	ECHA
Partition Coefficient (log K_{ow})	< -1.3 @ 20°C*	1	ECHA
Water Solubility	100 g/L @ 25 °C	-	ECHA

Cellulases, as pure enzyme, are white crystals or powder (HERA, 2005). An octanol-water partition coefficient (K_{ow}) for cellulase enzymes is not available. However, the log K_{ow} of glucoamylase, which cleaves 1,4–α-D-glycosidic linkages, was experimentally determined to be <1.3 at 20°C (ECHA). [Kl. score = 1]

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for hemicellulase enzymes.

Based on an assessment of environmental hazards, NICNAS identified hemicellulase enzymes as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

No information was located on the environmental fate of hemicellulase enzymes. Cellulase enzymes are readily biodegradable and are expected not to bioaccumulate or adsorb to soil.

Hemicellulase enzymes and other enzymes in this group are produced and destroyed within all terrestrial and aquatic ecosystems. They are ubiquitous, naturally occurring proteins which play important roles in the degradation of plant biomass and dissolved organic matter (DoEE, 2017a).

B. Biodegradation

No information is available on the hemicellulase enzymes.

A cellulase enzyme was readily biodegradable in an OECD 301F test. There was approximately 10% degradation after one day; approximately 60% after 5 days; and 129% after 28 days (ECHA). [Kl. score = 1]

Three different cellulase enzymes were considered readily biodegradable based on the results of OECD 301C and 301E tests (HERA, 2005) [Kl. scores = 1]. In an OECD 301E test, there was 84% DOC removal of the enzyme Carezyme after 28 days. In another OECD 301E test, there was 92% DOC removal of the enzyme Clazinase® after 28 days. In an OECD 301C test, BOD/COD was 78% after 28 days (HERA, 2005).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017b).

C. Environmental Distribution

Proteins, such as the hemicellulase enzymes, would not be expected to adsorb to soil. HERA (2005) listed a K_{oc} value of <1.3 for detergent amylases, cellulases and lipases that was calculated according to the EU Technical Guidance Document (EC, 2003). No further information was provided.

If released to water, based on its low K_{oc} and high water solubility values, cellulase is likely to remain in water and not adsorb to sediment. It is expected that they will rapidly denature in the aquatic environment and will be degraded by organisms and extracellular enzymes naturally present in aquatic ecosystems (DoEE, 2017a).

D. Bioaccumulation

No bioaccumulation studies were located on the hemicellulase enzymes. Hemicellulase enzymes are not expected to bioaccumulate due to their high molecular weight and their low K_{ow}. Moreover, hemicellulases are rapidly biotransformed in organisms to lower molecular-weight protein fragments by proteolytic enzymes (proteases), and eventually to the basic amino acids by peptidase enzymes.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No information is available on the hemicellulase enzymes. Cellulase enzymes have a moderate acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

No information is available on the hemicellulase enzymes. Table 2 lists the results of acute aquatic toxicity studies on the cellulase enzymes.

Table 2 Acute Aquatic Toxicity Studies on Cellulase Enzymes

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	>100* >52.1**	1	ECHA
Brachydanio rerio	96-hour LC_{50}	330*	4	HERA (2005)
Daphnia magna	48-hour EC_{50}	>100* >52.1**	1	ECHA
Daphnia magna	48-hour EC_{50}	>1,000**	4	HERA (2005)
Daphnia magna	48-hour EC_{50}	1,000**	4	HERA (2005)
Pseudokirchneriella subcapitata	72-hour EC_{50}	>100* >52.1**	1	ECHA
Scenedesmus subspicatus	72-hour EC_{50}	>1,000**	4	HERA (2005)

*Total organic solids.
**Active enzyme protein.

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Hemicellulase enzymes are expected to be readily biodegradable based on data from cellulase enzyme studies; thus, it does not meet the screening criteria for persistence.

Hemicellulase enzymes have a high molecular weight, hydrophilic properties (high water solubility, log K_{ow} <1.3) and are readily biotransformed in organisms by proteases and peptidases. Thus, hemicellulase enzymes do not meet the screening criteria for bioaccumulation.

There are no aquatic toxicity studies on the hemicellulase enzymes. The acute EC_{50} values on the cellulase enzymes are >1 mg/L in fish, invertebrates and algae. Thus, the hemicellulase enzymes are not expected to meet the criteria for toxicity.

The overall conclusion is that the hemicellulase enzymes are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for hemicellulase enzymes.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hemicellulase Enzymes	9025-56-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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A. Abbreviations and Acronyms

°C	degrees Celsius
aep	active enzyme protein
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
COD	Chemical oxygen demand
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Cooperation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemical Substances
SGG	Synthetic Greenhouse Gases

HETEROCYCLIC POLYMER CONTAINING NITROGEN COMPOUNDS (POLYVINYLPYRROLIDONE-PVP)

This dossier on heterocyclic polymer containing nitrogen compounds or polyvinylpyrrolidone (PVP) presents the most critical studies pertinent to the risk assessment of these substances in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Heterocyclic polymer containing nitrogen compounds is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Heterocyclic polymer containing nitrogen compounds, also known as polyvinylpyrrolidone (or commonly called polyvidone or povidone), is a water-soluble polymer made from the monomer N-vinylpyrrolidone. The substance appears on the Union list of authorised monomers, other starting substances, macromolecules obtained from microbial fermentation, additives and polymer production aids intended to come into contact with food. The U.S. Food and Drug Administration (FDA) has approved this chemical for many uses, and it is generally recognized as safe. The polymer is typically used as a pharmaceutical aid, complexing agent, and a solubilizer.

PVP is expected to degrade and has a low tendency to bind to soil or sediment. It is not expected to bioaccumulate. PVP is expected to be of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1-ethenylpyrrolidin-2-one

CAS RN: 9003-39-8

Molecular formula: $(C_6H_9NO)_n$

Molecular weight: 2,500 – 2,500,000 g/mol

Synonyms: PVP, Povidone, PVPP, Crospovidone, Polyvidone, PNVP, Poly[1-(2-oxo-1-pyrrolidinyl)ethylen], 1-Ethenyl-2-pyrrolidon homopolymer, 1-Vinyl-2-pyrrolidinon-Polymere

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of PVP

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White powder	-	PubChem
Melting Point	139°C (pressure not provided)	-	PubChem
Boiling Point	90-93°C @ 1.3 kPa	-	PubChem
Density	1230 – 1290 kg/m³ @ 25°C	-	PubChem
Vapour Pressure	12 Pa @ 20°C	-	PubChem
Partition Coefficient (log K_{ow})	0.4 (pH and temperature not provided)	-	PubChem
Water Solubility	>100 g/L @ 20°C	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for PVP.

NICNAS has assessed PVP in an IMAP Tier 1 assessment and considers it a polymer of low concern[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

PVP is expected to degrade and has a low tendency to bind to soil or sediment. It is not expected to bioaccumulate.

B. Biodegradation

PVP is a member of the family of hydrosoluble biomaterials: poly(N-vinyl-2-pyrrolidone) (PVP)-based graft copolymers. A synthesis route has been elaborated in which ω-functionalized PVP is prepared via chain-transfer radical polymerization, end-group modified, and subsequently grafted onto a polyhydroxylated backbone, typically dextran or poly(vinyl alcohol). The resulting graft copolymer biomaterials are designed for use in various biomedical applications, particularly as materials with a stronger potential for plasma expansion than already existing products have. The graft copolymers are potentially degradable because the PVP grafts are connected to the polyol backbone via a hydrolytically labile carbonate or ester linkage (Brunius et. al. 2002).

Overall, PVP is expected to degrade in the environment.

C. Environmental Distribution

No studies were available for the substance. Based on a log K_{ow} of 0.4, the substance is expected to have a low potential for adsorption and have very high mobility in soil. If released to water, based on its high water solubility value, it is likely to remain in water and not adsorb to suspended solids or sediment.

D. Bioaccumulation

No studies were available as the substance. Aliphatic alcohol ethoxylate has a low K_{ow} (0.44); and, therefore, bioaccumulation is expected to be low.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

PVP is expected to be of low toxicity concern to aquatic and terrestrial organisms. Details are provided below.

B. Aquatic Toxicity

<u>Acute Studies</u>

PVP has limited aquatic toxicity data. A 96-hour LC_{50} value for fish (*Scopthalmus maximus*) has been reported to be >1000 mg/L (Inveresk Research International, 1995).

<u>Chronic Studies</u>

No studies were available. However, given the large molecular weight of PVP, uptake and significant toxicity is not expected.

C. Terrestrial Toxicity

No studies were available. However, given the large molecular weight of PVP, uptake and significant toxicity is not expected.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Significant biodegradation of PVP is expected. For the purposes of this PBT assessment, the persistence criterion is not met.

The low K_{ow} of the substance suggests that bioaccumulation is not a concern. Therefore, the screening criteria for bioaccumulation is not met.

There are no chronic aquatic toxicity data available on PVP. The acute LC_{50} values > 1 mg/L. Thus, PVP does not meet the screening criteria for toxicity.

The overall conclusion is that PVP is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for PVP.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Heterocyclic polymer containing nitrogen compounds	9003-39-8	Not a PBT	No	Yes	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

6. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration

mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
PEC	Predicted exposure concentrations
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

HEXAMETHYLENEDIAMINE

This dossier on hexamethylenediamine (HMD) presents the most critical studies pertinent to the risk assessment of HMD in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – HMD is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

HMD is an aliphatic amine that is a colourless to white mass crystallised solid at ambient temperatures; however, it is typically handled in industrial applications as a liquid (ECHA).

HMD is readily biodegradable. It is not expected to bioaccumulate, and accumulation in soil or sediment is not to be expected. HMD exhibits low acute and chronic toxicity to aquatic organisms. Terrestrial toxicity is not of concern.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): hexane-1,6-diamine

CAS RN: 124-09-4

Molecular formula: $C_6H_{16}N_2$

Molecular weight: 116.20 g/mol

Synonyms: hexamethylenediamine; 1,6-hexanediamine; 1,6-diaminohexane; 1,6-diaminohexamethylene; 1,6-hexamethylenediamine

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Hexamethylenediamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	colourless to white crystallized mass	2	ECHA
Melting Point	36-43 °C @ 101.3 kPa:	2	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	201 °C @ 101.3 kPa		
Density	978 kg/m^3 @ 20°C	1	ECHA
Vapor Pressure	1000 Pa @ 78.5°C	1	ECHA
Partition Coefficient (log K_{ow})	0.4 (unionised form, at pH >= 13)	1	ECHA
Water Solubility	637 g/L@ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for HMD.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

HMD is readily biodegradable. It is not expected to bioaccumulate, and accumulation in soil or sediment is not to be expected.

B. Partitioning

HMD is highly soluble in water. Volatilization from water or moist soil surfaces is not expected to be an important fate process based upon its Henry's Law Constant (3.26 x 10^{-4} Pa m^3/mol). It is also not expected to volatilize from dry soil surfaces based upon its estimated vapour pressure.

C. Biodegradation

HMD is readily biodegradable. In an OECD 301D closed bottle test, there was 40% degradation after 7 days, 74% after 14 days, and 82% after 28 days (ECHA) [Kl. Score = 1]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

While HMD is highly hydrophilic (log P_{ow} <=0.4) and does not show surface active properties, aliphatic amines are strong bases and are protonated at environmental pH and, in consequence, due to the positive charge are prone to bind on negatively charged solid matter. This is demonstrated by the results from the available adsorption-desorption study (OECD 106): The bifunctional aliphatic amine HMD (2 amino groups) turned out to bind to soil and - to a lower level - sediment. The K_{oc} for HMD was calculated to be between 14 L/kg and 714 L/kg. Binding was not a function of organic carbon content of the soils. Rather, clay and silt content might be decisive. Desorption was observed and was considerable, but extent of desorption declined over time. Due to the observed rapid mineralization, accumulation in soil or sediment is not to be expected. (ECHA). [Kl. score = 1]

E. Bioaccumulation

In accordance with column 2 of Annex IX 9.3.2 of REACH Regulation EC 1907/2006 (ECHA), bioaccumulation testing in aquatic species is not required as the substance has a low potential for bioaccumulation (log K_{ow} of < 3).

The log K_{ow} for HMD is 0.4. Thus, HMD is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

HMD exhibits low acute and chronic toxicity to aquatic organisms. Terrestrial toxicity is not of concern.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on salts of hexamethylenediamine.

Table 3: Acute Aquatic Toxicity Studies on hexamethylenediamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Freshwater fish	96-hr LC50	1,825	2	ECHA
Daphnia magna	48-hr EC50	31.5	2	ECHA
Freshwater algae	72-hr EC50	>100	2	ECHA

Chronic Studies

Chronic data of good reliability from international guidelines are available for algae and invertebrates. The lowest value is a NOEC of 4.2 mg/L based on a 21-day reproduction test on daphnids performed according to the OECD 211 Guideline (ECHA) [Kl. Score = 4]. A chronic fish study

has been waived due to the much lower sensitivity of this trophic level compared to the daphnid data.

C. Terrestrial Toxicity

Terrestrial toxicity of the submission substance was analyzed with regard to earthworm reproduction according to OECD 222 and ISO 11268-2 (Part 2), compliant with GLP (RL 1). The earthworm Eisenia fetida (Lumbricidae) was chosen as a representative of the soil fauna.

The EC10 was calculated as 176.1 mg test item/kg soil (dw) (95% Confidence limits (CL) = 151.0 – 202.3 mg test item/kg soil (dw)).

The EC50 was calculated as 441.9 mg test item/kg soil (dw) (95% CL = 414.3 – 475.3 mg test item/kg soil (dw)).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

HMD is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The log K_{ow} for HMD is 0.4. Thus, HMD does not meet the screening criteria for bioaccumulation.

The NOEC values from chronic aquatic toxicity studies on HMD is >0.1 mg/L. The acute aquatic toxicity E(L)C50 values for HMD are > 1 mg/L. Thus, HMD does not meet the screening criteria for toxicity.

The overall conclusion is that HMD is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for HMD.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hexamethylenediamine	124-09-4	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy (DoEE). (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

Hexanedinitrile

This dossier on hexanedinitrile presents the most critical studies pertinent to the risk assessment of hexanedinitrile in its use in drilling muds. Sufficient data does not exist for this particular substance. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from The National Industrial Chemicals Notification and Assessment Scheme (NICNAS, 1994) and the ECHA database that provides information on chemicals that have been registered under the European Union (EU) REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Hexanedinitrile is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Hexanedinitrile, also known as adiponitrile, is used as a clay inhibitor. It is readily biodegradable and has low potential to bioaccumulate or to absorb to soil. Hexanedinitrile is of low acute toxicity concern to aquatic life. Chronic aquatic toxicity studies were not available.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Hexanedinitrile

CAS RN: 111-69-3

Molecular formula: $C_6H_8N_2$

Molecular weight: 108.14 g/mol

Synonyms: 1,4-Dicyanobutane, adipodinitrile

3 PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of Physico-Chemical Properties of Hexanedinitrile

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Slightly brown liquid	1	ECHA
Melting Point	-5 °C to 6°C[1]	1	ECHA
Boiling Point	305.3°C @ 99.5 kPa	1	ECHA
Density	968 Kg/m^3@ 20°C	2	ECHA
Vapour Pressure	0.091 Pa @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	-0.32 @ 25°C	2	ECHA
Water Solubility	80 g/L @ 20°C	2	ECHA

[1] No information on the atmospheric pressure reported.

Property	Value	Klimisch score	Reference
Viscosity	58 mPa s @30°C	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for hexanedinitrile.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Hexanedinitrile is expected to readily degrade. It is not expected to bioaccumulate, and it has a low potential to adsorb to soil.

B. Partitioning

Hexanedinitrile is highly soluble in water. Volatilisation from water surfaces or moist soil surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. It is also not expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

C. Biodegradation

A closed bottle test was conducted according to OECD 301 (2009) and the result was noted as inherently biodegradable (ECHA) (KI Score = 2). No specific data on degradation rates were provided.

Another test was conducted according to OECD 301A (2002) and the result was noted as rapidly biodegradable (ECHA) (KI Score=1). No specific data on degradation rates were provided.

Based on the summarized data above, the USEPA EPISuite BIOWIN7 (Anaerobic Linear Model) was used to estimate the probability of ready biodegradability. The results of the modelling indicated that the substance has a high probability (0.94) of ready biodegradation.

Therefore, the weight of evidence suggests that the substance in readily degradable.

If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No data were available on the adsorption/desorption properties of the substance.

Based on the lack of data for this parameter, USEPA EPISuite KOCWIN v2.00 was used to estimate the log K_{oc} of 1.305 using the molecular connectivity index (MCI) methodology. Based on this estimated value, hexanedintrile is expected to have very high mobility in soil. If released to water, based on the log K_{oc} value and its high water solubility, it is also not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

No data are available for the substance. Based on the lack of data available, USEPA EPISuite BCFBAF v 3.01 was used to estimate bioaccumulation based on the above noted log K_{ow} of -0.32 (Table 1). The modelled log bioconcentration factor (BCF) is equal to 0.5. Overall, the substance is not expected to bioaccumulate to a substantial degree based on the low log K_{ow} and predicted low log BCF.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Hexanedinitrile is of low acute toxicity potential to aquatic organism.

B. Aquatic Toxicity

Table 3 lists the results of acute aquatic toxicity studies on hexanedinitrile. It is expected to be readily biodegradable and is not expected to bioaccumulate.

Table 3 Acute Aquatic Toxicity Studies Hexanedinitrile

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Freshwater Fish[a]	96-hr LC_{50}	670	-	ECHA
Freshwater invertebrates[a]	48-hr EC_{50}	1189	-	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50} NOEC	>97.4	1	ECHA

a – Species not provided in study summary

No chronic studies were available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

Hexanedinitrile is readily biodegradable in the aquatic environment; thus, it does not meet the screening criteria for persistence.

The measured log K_{ow} for the substance is -0.32. Based on the calculated bioaccumulation factor of 0.5, hexanedinitrile is not bioaccumulative.

Acute toxicity for aquatic receptors across three tropic levels is > 1mg/L. Therefore, the substance does not fulfill the toxicity criterion.

The overall conclusion is that hexanedinitrile is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for hexanedinitrile.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hexanedinitrile	111-69-3	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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PubChem. National Institutes of Health. National Library of Medicine National Center for Biotechnology Information. https://pubchem.ncbi.nlm.nih.gov/

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
atm-cu m/mole	
BCF	bioconcentration factor
COC	constituent of concern
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mL	grams per millilitre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal

LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mm	millimetre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

HYDROXYPROPYL GUAR

This dossier on does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies pertinent to the risk assessment of hydroxypropyl guar in its use in coal seam gas extraction activities. The information presented in this dossier was obtained primarily from the United States Environmental Protection Agency (USEPA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Hydroxypropyl guar is classified as a **tier 1** chemical and requires a hazard assessment only.

1. BACKGROUND

Hydroxypropyl guar (HPG) is commonly used as a thickener of hydraulic fracturing fluid. It is also used as an inert ingredient as a thickener in pesticide formulations applied to growing crops only; as an indirect food additive; and, as a sizing agent in textiles/papers.

The substance is a propylene glycol ether derivative of guar gum. Guar gum is a resinous material derived from milled endosperm from guar beans of the legume *Cyamopsis tetragonolobus*. Structurally, it is a galactomannan (high molecular weight carbohydrate polymer) consisting of a main chain of D-mannose with a side chain of D-galactose at approximately every second mannose unit. The mannose units are β-(l-4) linked, and the single D-galactose units are joined to the main chain by α-(1-6) linkages.

Hydroxypropyl guar is readily biodegradable and is not expected to bioaccumulate. Based on its high molecular weight and polysaccharide structure, the substance would be expected to be of low acute and chronic toxicity to aquatic organisms.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Guar gum, 2-hydroxypropyl ether

CAS RN: 39421-75-5

Molecular formula: $(C_3H_8O_2)x$ (UVCB substance)

Molecular weight: 536.4362 g/mol; 200,000 to 300,000 daltons (Glickman, 1969) (UVCB substance)

Synonyms: Hydroxypropyl guar; hydroxypropyl guar gum; guar gum, 2-hydroxypropyl ether

3. PHYSIO-CHEMICAL PROPERTIES

Hydroxypropyl guar is a white to yellow fine powder that is very slightly soluble in water. It is a polysaccharide comprised of a polymannose backbone with mono-galactose pendent groups (whereby the mannose:galactose ratio is 2:1), derivatized via ether linkages with propylene glycol, at some of the free hydroxyl groups of the polysaccharide backbone (Johnson et al., 2015).

Hydroxypropyl guar is a slightly modified form of guar gum. Guar gum's polymeric structure contains numerous hydroxyl groups, which can be treated to form propylene glycol ethers, resulting in hydroxypropyl guar gum. As is the case with the hydroxypropyl derivatives of cellulose and methylcellulose, this modification has an impact upon the viscosifying properties of the polymer (which makes it more desirable for certain commercial applications) but does not increase toxicological concerns (USEPA, 2005).

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for hydroxylpropyl guar.

NICNAS has assessed hydroxypropyl guar in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5. ENVIRONMENTAL FATE SUMMARY

As a high molecular weight polysaccharide biopolymer, hydroxypropyl guar is readily biodegradable with microbial degradation being the major route of transformation in the environment. Adsorption onto soil and sediment particulates is very strong and, therefore, there is negligible potential to reach surface water by dissolved runoff and/or leach to ground water. Volatilization from soils and water is not likely to be a transport process in the environment. The potential to bioaccumulate is expected to be very low. (Kl Score = 3) (USEPA 2005).

6. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No toxicity data was available for review for this substance. However, USEPA concluded that hydroxypropyl guar, based on its high molecular weight and polysaccharide structure, would be

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=39421-75-5%2C+

expected to be of low acute and chronic toxicity to fish (fathead minnow), invertebrates (*Daphnia magna*) and green algae (*Selenastrum capriconutum*). Similarly, based on the high molecular weight and nonbioavailability of this substance, toxicity to terrestrial organisms is expected to be low (USEPA, 2005).

This conclusion is further supported by aquatic toxicity data available for parent compound guar gum (CAS No. 9000-30-0), which is provided below.

B. Aquatic Toxicity

The 96-hour LC_{50} for *Oncorhynchus mykiss* is 218 mg/L (Biesinger *et al.*, 1976). [Kl. score = 2]

The 48-hour and 96-hour LC_{50} values for *Daphnia magna* are 42 mg/L and <6.2 mg/L, respectively (Biesinger *et al.*, 1976). [Kl. score = 2]

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Hydroxypropyl guar is readily biodegradable and thus does not meet the screening criteria for persistence.

No bioconcentration studies are available for hydroxypropyl guar. Based on the large molecular weight of the biopolymer bioconcentration is not expected. Hydroxypropyl guar does not mee the screening criteria for bioaccumulation.

No toxicity data is available for hydroxypropyl guar. Based on a read across using parent compound guar gum, the 96-hour LC_{50} value for *Daphnia* is <6.2 mg/L. Thus, hydroxypropyl guar may potentially meet the screening criteria for toxicity.

The overall conclusion is that hydroxypropyl guar is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for hydroxypropyl guar.

8. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hydroxypropyl Guar	39421-75-5	Not a PBT	No	No	No	No	No	Potentially Yes	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). Based on a read-across to parent guar gum (CAS No. 9000-30-0).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development

PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

IRON OXIDE

This dossier on iron oxide presents the most critical studies pertinent to the risk assessment of iron oxide in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Iron oxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Iron oxide is an inorganic compound. It is partially soluble in water, dissociating into iron and hydroxyl ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. Iron oxide is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): diiron(3+) trioxidandiide

CAS RN: 1309-37-1

Molecular formula: Fe_2O_3

Molecular weight: 177.7 g/mol

Synonyms: Hydrous ferric oxide, Iron oxide (Fe_2O_3), hydrate iron (III) oxide monohydrate, Iron oxide (Fe_2O_3), hydrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Iron Oxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Red solid	1	ECHA
Melting Point	1,565 °C @ 101.3 kPa	1	ECHA
Boiling Point	In accordance with REACH Annex VII (ECHA), the study does not need to be conducted, as the substance has a melting point > 300°C.	1	ECHA
Density	5250 kg/m³ @ 25 °C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	In accordance with column 2 of REACH Annex VII (ECHA), the study does not need to be conducted, as the substance has a melting point above 300°C.	-	-
Partition Coefficient (log K_{ow})	In accordance with column 2 of REACH Annex VII (ECHA), the study does not need to be conducted as the substance is inorganic.	-	-
Water Solubility	With a loading of 10 g/L diiron trioxide to water at pH8 the dissolved iron was determined to be < 1 µg/L.	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for iron oxide.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Iron is relatively immobile under most environmental conditions, mainly due to the very low solubility of iron (III) hydroxide in its various forms (REACH). As an inorganic substance, iron oxide is expected to disassociate in the environment to its respective cation and anion as limited by its aqueous solubility and pH.

In soil, as well as in sediment-water systems, iron oxide will react and release iron ions and hydroxyl ions. Therefore, relevant information on adsorption/desorption of iron oxide can be broadened to data on adsorption/desorption of iron and magnesium. The behaviour of hydroxyl ions depends on the pH buffer capacity of the tested medium. The pH buffer capacity is controlled by a whole range of processes (mineral dissolution/precipitation, protonation/deprotonation of pH dependent charge

sites, reaction with CO_2, biological processes, etc.) and as such, partition coefficients are not relevant for the fate and behaviour of OH- in soils or sediment.

For iron an essential, homeostatically controlled element, the bioaccumulation potential is considered to be low. A similarly low potential is assumed for the poorly soluble iron oxide (REACH).

6 ENVIRONMENTAL EFFECTS SUMMARY

As based on the physico-chemical properties and its extremely low water solubility, the substances of the "Iron Oxides Category" (iron oxides) are expected to have a low potential for adsorption, and studies on adsorption / desorption do not need to be conducted. All category members are ubiquitous in the environment. Iron, manganese and zinc are essential elements for humans, animals, plants and microorganisms. The Henry's law constant (HLC) and the distribution of iron oxides in the environment are not calculated according to the Mackay fugacity model, because the substances are inorganic and have an extremely low vapour pressure at ambient temperature. Iron oxides are not volatile from aqueous suspensions. In the atmosphere, iron oxide substances will exist solely in the particulate phase and may be removed from the air by wet and dry deposition.

A. Summary

Iron oxide is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on iron oxide.

Table 3 Acute Aquatic Toxicity Studies on Iron Oxide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachydanio rerio	96-hour LC_{50}	>/= 50000 mg/L	1	ECHA
Daphnia magna	48-hour EC_{50}	>/= 100 mg/L	1	ECHA

Chronic Studies

In accordance with section 1 of REACH Annex XI (ECHA), the study on long-term toxicity to fish does not need to be conducted. Natural baseline iron concentrations in the aquatic environment are already much higher than the reported saturation concentrations of iron oxides in the environment. As such, it is unlikely that iron ions released from iron oxides would inhibit growth and proliferation of aquatic plants, animals or microorganisms.

C. Terrestrial Toxicity

No data are available on the effects of iron oxides on terrestrial organisms. Iron is ubiquitous in the environment. It comprises some 5% of the earth's crust. Iron oxides are widespread in soils. Iron occurs mostly in the form of its oxides. The predominant iron mineral in soils is goethite (alpha-FeOOH). The most important iron ores are magnetite (Fe_3O_4) and hematite (alpha-Fe_2O_3).

The interstitial water of the soil is in contact with natural iron oxide minerals. Its concentrations of iron-, manganese- and zinc ions depend on several environmental factors (e.g. duration of contact, temperature and presence of humic substances) and natural complexions (e.g. siderophores). Input of iron oxide pigments will not increase the "saturation" concentrations, and it is very unlikely that synthetic pigments have any significant effect on ion contents in soil water or on other soil properties. On the other hand, if the iron oxides would increase the soil content of iron-, manganese- and zinc ions, this would be a fertilizing effect in line with the purpose of sewage sludge application on agricultural land.

Performing a test is scientifically not necessary, as the category members are inert inorganic oxides of iron which resemble naturally occurring iron oxides. Even under worst case conditions, an inhibitory effect of synthetic iron oxide pigments is not likely to be exerted on soil organisms.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Iron oxide is an organic salt that dissociates to iron and hydroxyl ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both iron and hydroxyl ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Acute aquatic toxicity data are >1 mg/L. There are no chronic toxicity data for this substance. Thus, iron oxide does not meet the screening criteria for toxicity.

The overall conclusion is that iron oxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for iron oxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Iron oxide	1309-37-1	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HLC	Henry's law constant
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
µg/L	micrograms per litre

ISOPROPANOL

This dossier on isopropanol presents the most critical studies pertinent to the risk assessment of isopropanol in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Isopropanol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Isopropanol is readily biodegradable, and it is not expected to bioaccumulate. It has a low tendency to bind to soil or sediment. Isopropanol is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Propan-2-ol

CAS RN: 67-63-0

Molecular formula: C_3H_8O

Molecular weight: 60.1 g/mol

Synonyms: Isopropanol, isopropyl alcohol, 2-propanol, *sec*-propyl alcohol, dimethylcarbinol

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Isopropanol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid	2	ECHA
Melting Point	-88.5°C; -89.5°C[1]	2	ECHA
Boiling Point	82.5°C; 82.3°C @ 101.3 kPa	2	ECHA
Density	800 Kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	4400 Pa @ 20°C; 6002 Pa @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	0.05 @ 25°C	2	ECHA
Water Solubility	Miscible	2	ECHA
Viscosity	2.038 mPa s @ 25°C	2	ECHA

[1] No information on the atmospheric pressure reported.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for isopropanol.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Isopropanol is readily biodegradable. It is not expected to bioaccumulate. Isopropanol has a low tendency to bind to soil or sediment.

B. Partitioning

Isopropanol is miscible in water. Volatilisation from water surfaces or moist soil surfaces is expected to be an important fate process based upon this compound's estimated Henry's Law constant of 0.821 Pa m^3/mole. It is also expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

C. Biodegradation

Aerobic biodegradation of isopropanol has been shown to occur rapidly under non-acclimated conditions, based on a result of 49% biodegradation from a 5-day BOD test (Bridie *et al.*, 1979). Additional biodegradation data developed using standardised test methods show that isopropanol is readily biodegradable in both freshwater and saltwater media (72 to 78% biodegradation in 20 days) (Price *et al.*, 1974).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for isopropanol. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 3.478 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 1.53 L/kg.

E. Bioaccumulation

Bioconcentration of isopropanol in aquatic organisms is not expected to occur based on a measured log K_{ow} of 0.05 (ECHA). Based on this estimated value, the substance is expected to have very high mobility in soil. If released to water, based on this value and its water solubility, it is also not expected to adsorb to suspended solids and sediment.

Volatilisation from water surfaces is expected with half-lives for a model river and model lake of 86 hours and 29 days, respectively (PubChem).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Isopropanol is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on isopropanol.

Table 3 Acute Aquatic Toxicity Studies on Isopropanol

Test Species	Endpoint	Results	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	9,640 mg/L	2	ECHA
Daphnia magna	24-hour EC_{50}	>10,000 mg/L	2	ECHA

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies on diethanolamine.

Table 4 Chronic Aquatic Toxicity Studies on Isopropanol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	16-day NOEC	141 mg/L	4	ECHA
Daphnia magna	21-day NOEC	30 mg/L	4	OECD, 1977a,b
Scenedesmus quadricauda	7-day NOEC	1,800 mg/L	2	ECHA

C. Terrestrial Toxicity

An EC_{50} value of 2,100 mg/L was determined from a lettuce seed germination test (Reynold, 1977) [Kl. score = 2].

7 CATEGORISATION AND OTHER CHARCTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Isopropanol is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 0.05 and a calculated BCF of 1, isopropanol does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on isopropanol show a NOEC of >0.1 mg/L. The acute EC_{50} values for isopropanol in fish, invertebrates and algae are >1 mg/L. Thus, isopropanol does not meet the screening criteria for toxicity.

The overall conclusion is that isopropanol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for isopropanol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Isopropanol	67-63-0	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BOD	Biological oxygen demand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA modelling program to estimate the organic carbon-normalised sorption coefficient for soil and sediment
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second

NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

LACTOSE

This dossier on lactose presents the most critical studies pertinent to the risk assessment of lactose in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Lactose is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Lactose is a disaccharide sugar composed of galactose and glucose. It is naturally synthesised in the mammary gland of virtually all mammals, occurring in milk at levels between 1 and 7%. No biodegradation studies were found on lactose. As a disaccharide of galactose and glucose sugars, lactose would be expected to be readily biodegradable. It would also not be expected to bioaccumulate or adsorb to sediments or soil. Lactose is expected to be of low toxicity concern to aquatic organisms based on QSAR modelling results.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): β-D-galacto-hexopyranosyl-(1→4)-α-D-glucose

CAS RN: 63-42-3

Molecular formula: $C_{12}H_{22}O_{11}$

Molecular weight: 342.3 g/mol

Synonyms: Lactose; alpha-lactose; lactose anhydrous; β-D-galacto-hexopyranosyl-(1->4)-α-D-gluco-hexopyranose; β-D-galactopyranosyl-4)-α-D-glucopyranose; α-D-glucopyranose, 4-O- β-D-galactopyranosyl-

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Lactose

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline powder	4	Lide (2007)
Melting Point	254°C[1]	4	Lide (2007)
Density	1590 Kg/m^3 @ 20°C	4	Lide (2007)

[1] No information on the atmospheric pressure reported.

Property	Value	Klimisch score	Reference
Vapour Pressure	4.56 x 10^{-14} Pa @ 25 °C	-	PubChem
Partition Coefficient (log K_{ow})	-5.03 (estimated)	-	USEPA (2017)
Water Solubility	1950 g/L @ @ 20°C	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for lactose.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Lactose is highly soluble in water. No biodegradation studies were found on lactose. However, as a disaccharide of galactose and glucose sugars, lactose would be expected to be readily biodegradable. It would also not be expected to bioaccumulate.

Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values from the molecular connectivity index (MCI) is 1 L/kg. Based on this estimated value, lactose is expected to have very high mobility in soil. If released to water, based on the estimated K_{oc} value and its high water solubility, it is also not expected to adsorb to suspended solids and sediment.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Lactose is expected to be of low toxicity concern to aquatic organisms based on QSAR modelling results.

B. Aquatic Toxicity

Acute Studies

No aquatic toxicity studies were found on lactose.

Using the ECOSAR module of EPISUITE, the 96-hour LC_{50} in fish was estimated to be 93,396 mg/L; the 48-hour LC_{50} in *Daphnia* and the 96-hour EC_{50} in green algae exceed the estimated water solubility of 111,000 mg/L (USEPA, 2017).

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

No biodegradation data are available on lactose. Lactose is a disaccharide found in milk and consists of D-galactose and D-glucose sugars. it is expected to be readily biodegradable; therefore, it does not meet the screening criteria for persistence.

Lactose is a disaccharide that has an estimated log K_{ow} of -5. It is water-soluble and is rapidly metabolised by enzymes. It is not expected to bioaccumulate.

The estimated acute EC_{50} value in fish is >1 mg/L. Thus it does not meet the screening criteria for toxicity.

The overall conclusion is that lactose is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for lactose.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Lactose	63-42-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
ECOSAR	USEPA modelling program to estimate aquatic toxicity
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre

KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

LECITHIN

This dossier on lecithin presents the most critical studies pertinent to the risk assessment of lecithin in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the U.S. Cosmetic Ingredient Review on lecithin (CIR, 2001). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Lecithin is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Lecithin is a naturally occurring mixture of the diglycerides of stearic, palmitic and oleic acids, linked to the choline ester of phosphoric acid; it is found in living plants and animals. Lecithin is a UVCB substance. No studies are available. Lecithin is found in all living organisms; it is expected to be readily biodegradable and with no potential for bioaccumulation. No studies are available to evaluate the environmental hazard of lecithin however based on its biological essentiality it is not expected to be substantially toxic to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Lecithin

CAS RN: 8002-43-5

Molecular formula: $C_{43}H_{88}NO_9P$ (approximate) [CIR, 2001]

Molecular weight: 144.56 g/mol [CIR, 2001]

Synonyms: Lecithin, egg yolk lecithin; lecithins, egg yolk; lecithin, soybean; soybean phospholipid; lecithol: phosphatidylcholine; choline phospshoglyceride; and phospholutein

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Lecithin

Property	Value	Reference
Physical state at 20°C and 101.3 kPa	Natural and refined grades vary from plastic to fluid, depending on free fatty acid and oil content and on the presence/absence of other diluents. Light yellow to brown. Amber, viscous liquid.	CIR, 2001
Melting Point	236 – 237°C[1]	CIR, 2001

[1] No information on the atmospheric pressure reported.

Property	Value	Reference
Specific Gravity	1.0305 @ 24°C; 1.02-1.06 @ 25°C	CIR, 2001
Solubility	Insoluble in water; partially soluble in water – readily hydrates to form emulsions.	CIR, 2001

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for lecithin.

NICNAS has assessed lecithin in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[2] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No studies are available. Lecithin is found in all living organisms; it is expected to be readily biodegradable and with no potential for bioaccumulation. In mixed micelles, degradation almost exclusively affects the lecithin component through hydrolysis into free fatty acids and lysolecithin. Lecithins oxidise rapidly on exposure to air (CIR, 2001).

6 ENVIRONMENTAL EFFECTS SUMMARY

No relevant aquatic acute or chronic toxicity studies are available.

Physiological effects of lecithin in feed have been studied in aquatic animals. Purified deoiled dry forms of lecithin are used as supplements in aquaculture to enhance growth in early stages of development (Meyers, 1995).

[2] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=8002-43-5

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Lecithin is a phospholipid that is found in living organisms. For example, it is a predominant phospholipid in membranes, in egg yolk, lung surfactant and amniotic fluid. Although there are no biodegradation studies on lecithin, it is expected to be readily biodegradable; thus it does not meet the screening criteria for persistence.

Lecithin is a naturally occurring phospholipid found in living organisms. It is not expected to bioaccumulate.

There are no aquatic toxicity studies on lecithin. As a naturally occurring phospholipid, it is not expected to meet the criteria for toxicity.

The overall conclusion is that lecithin is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for lecithin.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Lecithin	8002-43-5	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency

EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
kPa	kilopascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

MAGNESIUM CHLORIDE

This dossier on magnesium chloride presents the most critical studies pertinent to the risk assessment of this substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Magnesium chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Magnesium chloride dissociates completely in water to the Mg++ cation and the chloride anion (Cl-). Biodegradation is not applicable to magnesium chloride. Magnesium chloride and its dissociated ions are ubiquitous in the environment; they are not expected to adsorb to soil or sediment or to bioaccumulate. Magnesium chloride is of low toxicity concern to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Magnesium (2+) dichloride

CAS RN: 7786-30-3

Molecular formula: Cl_2Mg

Molecular weight: 95.2 g/mol

Synonyms: Magnesium chloride; magnesium (2+) dichloride; magnesium chloride, anhydrous

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Magnesium Chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless or white hexagonal crystals	2	ECHA
Melting point	712°C @ 101.3 kPa	2	ECHA
Boiling point	1412 °C (pressure not provided)_	-	ECHA
Density	2316 kg/m^3 @ 20°C	1	ECHA
Water Solubility	468.7 g/L @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for magnesium chloride.

NICNAS has assessed magnesium chloride in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment provided that ANZECC water quality guidelines for physical and chemical stressors are not exceeded[1]. In addition, based on an assessment of human health and environmental hazards, NICNAS also identified magnesium chloride as a chemical of low concern to the environment (NICNAS, 2017 and DoEE, 2017). Chemicals of low concern are unlikely to have adverse environmental effects or be a concern to human health if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Given its high solubility in water, magnesium chloride will dissociate and release magnesium (Mg^{2+}) and chloride (Cl^-) ions. The dissociated Mg^{2+} cation can then transform and form complexes with dissolved ligands present in natural waters. Magnesium is widespread in living cells and does not bioconcentrate in aquatic organisms. Environmental fate analysis based on log Kow and log Koc and typical fugacity modelling is not applicable to magnesium chloride as it is an inorganic compound. Photodegradation and biodegradation are also not applicable to inorganic metal salts such as magnesium chloride (OECD, 2011).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Magnesium chloride is of low toxicity concern to aquatic life.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7786-30-3

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on magnesium chloride.

Table 3: Acute Aquatic Toxicity Studies on Magnesium Chloride

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hr LC_{50}	2,119	2	ECHA
Daphnia magna	48-hr LC_{50}	548	2	ECHA
Daphnia magna	48-hr LC_{50}	841	2	ECHA
Ceriodaphnia dubia	48-hr LC_{50}	1,328	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50} NOEC	>100 100	1	ECHA

Chronic Studies

The 21-day EC_{10} of magnesium chloride in a Daphnia reproduction test is 321 mg/L (ECHA) [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

Magnesium and chloride ions are ubiquitous in the environment and are found naturally in soil, water and sediment (Mg in soils/sediments are at a 50th percentile level in the range of 0.9-1.2 %). Magnesium will be assimilated by species residing in the soil and is necessary to maintain a good chemical balance in soils, water and sediment. The chloride will become part of the chloride cycle and/or be assimilated by microorganisms and other species that require chloride as an essential substance in their biological systems/ processes. Natural magnesium minerals are quite soluble, and so differences in bioavailability between natural magnesium sources and anthropogenic added magnesium are not expected. For these reasons, it is expected that magnesium chloride would not be toxic to soil organisms and hence, short-term and long-term toxicity tests to terrestrial organisms are scientifically unjustified (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Magnesium chloride is an inorganic salt that dissociates completely to magnesium and chloride ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Magnesium chloride is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Thus, the substance does not meet the screening criteria for bioaccumulation.

The EC_{10} value from a chronic Daphnia reproduction study is >0.1mg/L. The acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Thus, magnesium chloride does not meet the screening criteria for toxicity.

The overall conclusion is that magnesium chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for magnesium chloride.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Magnesium chloride	7786-30-3	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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Department of the Environment and Energy [DoEE]. (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration

ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effect concentration
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

MAGNESIUM NITRATE

This dossier on magnesium nitrate presents the most critical studies pertinent to the risk assessment of this substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Magnesium nitrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Magnesium nitrate dissociates completely in aqueous solutions to magnesium (Mg^{++}) and nitrate (NO_3^-) ions. Biodegradation is not applicable to magnesium nitrate. Magnesium nitrate and its dissociated ions are ubiquitous in the environment. They are not expected to adsorb to soil or sediment or to bioaccumulate. Magnesium nitrate is of low toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Magnesium dinitrate

CAS RN: 10377-60-3

Molecular formula: $Mg(NO_3)_2$ or MgN_2O_6

Molecular weight: 148.31 g/mol

Synonyms: Magnesium nitrate; magnesium dinitrate; nitric acid, magnesium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Magnesium Nitrate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	2	ECHA
Melting Point	ca. 95°C (as hexahydrate) @ 101.3 kPa	2	ECHA
Boiling Point	substance is a solid which decomposes before boiling	-	ECHA
Density	1460 kg/m3 (as hexahydrate) @ 20°C	2	ECHA
Vapour Pressure	0 Pa @ 20°C	1	ECHA
Partition Coefficient (log Kow)	Not applicable given that this substance is inorganic	-	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	Soluble (as dehydrate) Very soluble (as hexahydrate) 10 g/L @ 20°C	2	ECHA
Dissociation constant (pKa)	11.4 @ 25 °C Magnesium (II) ion 3.25 @ 25 °C Nitrous acid (HNO2)	2	ECHA

Magnesium nitrate or $Mg(NO_3)_2$ is a hydroscopic salt that quickly forms the hydrate ($Mg(NO_3)_2 \bullet 6H_2O$) in air.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for magnesium nitrate.

NICNAS has assessed magnesium nitrate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] . In addition, based on an assessment of human health hazards, NICNAS also identified magnesium nitrate as a chemical of low concern to human health (NICNAS, 2017). Chemicals of low concern are unlikely to be a concern to human health if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Under typical environmental conditions, magnesium nitrate is expected to dissolve in water and fully dissociate into magnesium (Mg^{++}) and nitrate (NO_3^-) ions. These ions have a number of important functions in the environment. Magnesium ions are ubiquitous in the environment and are essential for proper functioning of cells (Campbell et al. 1999). Nitrates form a pivotal part the global nitrogen cycle, and are an essential plant nutrient (Barsanti and Gualtieri 2010).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=10377-60-3

As naturally ubiquitous ions, these substances are present in all environmental compartments and subject to environmental transport processes. As a result, these substances are expected to move to soil, sediment or water compartments upon release (DoEE, 2017). Based on the high water solubility and the ionic nature, magnesium nitrate is not expected to adsorb or bioaccumulate to a significant extent (ECHA).

However, if released in high volumes, these ions could potentially cause physico-chemical stresses in aquatic environments by direct and indirect pathways. For example, release of large amounts of these soluble salts directly into waterways has the potential to directly cause adverse effects on aquatic life by increasing the salinity of the water body. Direct and indirect stress could also occur as the result of excessive levels of nitrate which can cause eutrophication. Eutrophication can lead to a decrease in dissolved oxygen to levels which are insufficient to sustain normal respiration by aquatic life. However, numerous natural biogeochemical mechanisms exist which tend to limit fluctuations in nutrient levels, which occur frequently in healthy aquatic ecosystems (DoEE, 2017).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Magnesium nitrate is of low toxicity concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

No reliable study with magnesium nitrate is available. Based on reliable studies with ammonium nitrate, potassium sodium nitrate and potassium nitrate, the 96hr-LC_{50} is >100 mg/L for fish. (ECHA) [Kl. Score = 2]. A reliable study with potassium nitrate showed an 48-hr EC_{50} of 490 mg/L for invertebrates. (ECHA) [Kl. Score = 2].

No reliable short-term studies are available for algae, since nitrates are known stimulants for algal growth at low concentrations.

Chronic Studies

No reliable study with magnesium nitrate is available. There are reliable 30-d growth rate and 32-d embryo-larval tests available for read-across substance sodium nitrate. In the 30-d growth rate test the NOEC for juvenile Topeka shiner was 268 mg/L (growth rate) and the NOEC for Fathead minnow was 58 mg/L (mortality). (ECHA) [Kl. Score = 2]. In the 32-d embryo-larval test, the NOEC to Fathead minnow was 157 mg/L based on growth rate (no effect on embryo survival). (ECHA) [Kl. Score = 2].

The ANZECC/ARMCANZ (2000) default guideline value for nitrate was erroneous. In the absence of an ANZG (2018) default guideline value, the "Grading" guideline values published in the report *Updating nitrate toxicity effects on freshwater aquatic species* was reviewed. In developing a “grading” water quality guideline for nitrate, ANZG reviewed the literature on both potassium nitrate and sodium nitrate and identified NOECs for 9 fish, 8 invertebrate, 4 amphibians and 1 algal species (NIWA, 2013). The dataset spans a 391-fold range in sensitivity, with lake trout (*Salvelinus namaycush*) the most sensitive, with a NOEC of 1.6 mg NO_3-N/L for both growth and development endpoints measured after a 146-day exposure. In general, the chronic data indicate higher exposure sensitivity for fish, although both fish and invertebrates show wide ranges in sensitivity. The most

sensitive invertebrate NOEC (a freshwater crayfish, *Astacus astacus*) was 9x less sensitive than the most sensitive fish NOEC. Rainbow trout, the mayfly *Deleatidium sp*., and juvenile inanga were all markedly less sensitive than the most sensitive species, lake trout (by a factor of 16x, 13x and 7x respectively).

C. Terrestrial Toxicity

No studies were located.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Magnesium nitrate is an inorganic salt that dissociates completely to magnesium and nitrate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Magnesium nitrate is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Thus, the substance does not meet the screening criteria for bioaccumulation..

Limited aquatic toxicity data exist on magnesium nitrate. Based on a read-across, the NOEC values in are >0.1 mg/L in fish and invertebrates. The acute E(L)C_{50} values are >1 mg/L in fish and invertebrates. Thus, magnesium nitrate does not meet the screening criteria for toxicity.

The overall conclusion is that magnesium nitrate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for magnesium nitrate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Magnesium nitrate	10377-60-3	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

ANZECC and ARMCANZ. (2000). Australia and New Zealand Environment and Conservation Council and Agriculture and Resource Management Council of Australia and New Zealand 2000, Australian and New Zealand Guidelines for Fresh and Marine Water Quality (Vol. 1), Australian Water Association, Artarmon, NSW.

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Department of the Environment and Energy [DoEE]. (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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National Institute of Water and Atmospheric Research [NIWA]. 2013. Updating Nitrate Toxicity Effects on Freshwater Aquatic Species. Prepared for Ministry of Building, Innovation and Employment. Report No. HAM2013-009. January 2013.

B. Acronyms and Glossary

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances

ANZG	Australian and New Zealand Guidelines
ANZECC	Australia and New Zealand Environment and Conservation Council
ARMCANZ	Agriculture and Resource Management Council of Australia and New Zealand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

MAGNESIUM OXIDE

This dossier on magnesium oxide presents the most critical studies pertinent to the risk assessment of magnesium oxide in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Magnesium oxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

MgO is one of the components in Portland cement in dry process plants. Additionally, magnesium, an essential element to most biological systems, is provided to soil and groundwater microbial populations during MgO-assisted metals remediation. Magnesium oxide is of low toxicological concern and is used for relief of heartburn and dyspepsia, as an antacid, magnesium supplement and as a short-term laxative. It is also used to improve symptoms of indigestion.

Magnesium oxide is of low toxicity concern to environmental receptors, In fact, magnesium oxide is used extensively in the soil and groundwater remediation, wastewater treatment, drinking water treatment, air emissions treatment and waste treatment industries for its acid buffering capacity and related effectiveness in stabilizing dissolved heavy metal species.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Oxomagnesium

CAS RN: 1309-48-4

Molecular formula: MgO

Molecular weight: 40.305 g/mol

Synonyms: Magnesia, oxomagnesium, Periclase, Seawater magnesia, Magnesium oxide, Causmag, Granmag, Maglite

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Magnesium Oxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid, hygroscopic fine white powder.	-	Pubchem

Property	Value	Klimisch score	Reference
Melting Point	2,800 °C[1]	-	Pubchem
Boiling Point	3,600 °C[1]	-	Pubchem
Density	3600 kg/m^3	-	Pubchem
Vapour Pressure	0 Pa @ 25°C	-	Pubchem
Partition Coefficient (log K_{ow})	not applicable	-	-
Water Solubility	Poorly soluble (i.e., 0.009% @ 86°F)	-	Pubchem
Viscosity	Not applicable	-	-

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for magnesium oxide.

NICNAS has assessed magnesium oxide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[2]. It was identified as an inorganic substance with low toxicity and/or low bioavailability. Low concern to the environment.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] No information on atmospheric pressure provided.
[2] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=1309-48-4

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Magnesium oxide is an inorganic substance that is not subject to biodegradation, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Biodegradation

Magnesium oxide is an inorganic substance. According to Annex VII of the REACH regulations (ECHA), biodegradation testing for inorganic chemicals is not required.

C. Environmental Distribution

As an inorganic substance, magnesium oxide is expected to disassociate in the environment to its respective cation and anion as limited by its aqueous solubility and pH.

In soil, as well as in sediment-water systems, magnesium oxide will react and release magnesium ions and hydroxyl ions. Therefore, relevant information on adsorption/desorption of magnesium oxide can be broadened to data on adsorption/desorption of magnesium. The behaviour of hydroxyl ions depends on the pH buffer capacity of the tested medium. The pH buffer capacity is controlled by a whole range of processes (mineral dissolution/precipitation, protonation/deprotonation of pH dependent charge sites, reaction with CO_2, biological processes, etc.) and as such, partition coefficients are not relevant for the fate and behaviour of OH- in soils or sediment.

D. Bioaccumulation

There are no bioaccumulation studies on magnesium oxide. Magnesium is an essential element in biological systems. Magnesium occurs typically as the Mg2+ ion. It is an essential mineral nutrient and is present in every cell type in every organism. For example, ATP (adenosine triphosphate), the main source of energy in cells, must bind to a magnesium ion in order to be biologically active. As such, magnesium plays a role in the stability of all polyphosphate compounds in the cells, including those associated with the synthesis of DNA and RNA.

Over 300 enzymes require the presence of magnesium ions for their catalytic action, including all enzymes utilising or synthesising ATP, or those that use other nucleotides to synthesise DNA and RNA.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Magnesium oxide is of low acute toxicity concern to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion.

B. Aquatic Toxicity

Acute Studies

No studies were available on magnesium oxide. Thus, **Table 3** presents the results of acute aquatic toxicity studies on the hydrated magnesium hydroxide.

Table 3 Acute Aquatic Toxicity Studies on Magnesium Hydroxide

Test Substance	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Magnesium hydroxide	*Pimephales promelas*	96-hour LC_{50}	306.79	2	ECHA
Magnesium hydroxide	*Daphnia magna*	96-hour EC_{50}	170.6	2	ECHA
Magnesium hydroxide	*Chlorella vulgaris*	72-hour EC_{50}	>100	2	ECHA

Acute aquatic toxicity studies on soluble magnesium salts also indicates low toxicity. Toxicity endpoints identified generally exceeded 100 mg/L (ECHA).

Chronic Studies

No studies are available. Long-term toxicity of fish and invertebrates is unlikely to occur based on the physico-chemical properties of magnesium hydroxide, the breakdown pathway of the substance and the fact that magnesium ions are ubiquitous in the natural environment.

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Magnesium oxide is an inorganic mineral. Thus, biodegradation is not applicable to this substance. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to magnesium oxide.

Magnesium oxide is a naturally inorganic substance, while magnesium is naturally found in eukaryotic and prokaryotic cells involved in multiple biochemical pathways. Thus, magnesium oxide does not meet the screening criteria for bioaccumulation.

The NOECs from the acute aquatic toxicity studies on magnesium hydroxide (a magnesium oxide surrogate) are greater than 100 mg/L. Thus magnesium oxide, does not meet the criteria for toxicity.

Thus, magnesium oxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for magnesium oxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Magnesium oxide	1309-48-4	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Pubchem. Open chemistry database at the National Institutes of Health (NIH). https://pubchem.ncbi.nlm.nih.gov/

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
°F	degrees Fahrenheit
AICS	Australian Inventory of Chemical Substances
ATP	adenosine triphoshphate
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DNA	deoxyribonucleic acid
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal

LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RNA	ribonucleic acid
SGG	Synthetic Greenhouse Gases

MAGNESIUM SILICATE HYDRATE (TALC)

This dossier on magnesium silicate hydrate (talc) presents the most critical studies pertinent to the risk assessment of this substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Magnesium silicate hydrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Magnesium silicate hydrate (talc) is a clay mineral, composed of hydrated magnesium silicate with the chemical formula $Mg_3Si_4O_{10}(OH)_2$. Magnesium silicate hydrate (talc) is an inorganic substance for which biodegradation is irrelevant. It will not bioaccumulate, has a low potential to adsorb to soil, and has low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): dioxosilane;oxomagnesium;hydrate

CAS RN: 14807-96-6

Molecular formula: $H_2Mg_3O_{12}Si_4$

Molecular weight: 379.27 g/mol

Synonyms: Talcum, oxosilanediol, trimagnesium; dioxido(oxo)silane; hydroxy-oxido-oxosilane, dioxosilane; oxomagnesium; hydrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Magnesium Silicate Hydrate (talc)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White solid odorless powder	2	ECHA
Melting Point	1,500 °C @ 101.3 kPa	2	ECHA
Boiling Point	This substance is a solid that melts above 300 °C	-	ECHA
Density	2700 kg/m³ @ 20°C	2	ECHA
Vapor Pressure	0 Pa at 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-9.4 @ 25°C	2	ECHA
Water Solubility	0.0001 g/L @ 25°C; insoluble in water	2	ECHA
Dissociation constant	ND because the substance is insoluble in water	-	ECHA

ND – not determined

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for magnesium silicate hydrate (talc).

NICNAS has assessed magnesium silicate hydrate (talc) in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health nor the environment[1]. In addition, based on an assessment of human health and environmental hazards, NICNAS also identified magnesium silicate hydrate (talc) as a chemical of low concern to the environment (NICNAS, 2017 and DoEE, 2017). Chemicals of low concern are unlikely to have adverse environmental effects or be a concern to human health if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Magnesium silicate hydrate (talc) is an inorganic substance for which biodegradation is irrelevant. Moreover, it will not bioaccumulate and has a low potential to adsorb to soil or sediment.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=14807-96-6%2C+

B. Biodegradation

As an inorganic substance, magnesium silicate hydrate (talc) will not biodegrade. Soil and sediment degradation studies are not considered to be applicable as the test material is essentially insoluble in water and consists of materials which occur naturally in these compartments (ECHA).

C. Environmental Distribution

Magnesium silicate hydrate (talc) is insoluble in water. The log K_{OC} of was estimated to be 1.5027 which is equal to a K_{OC} value of 31.82 L/kg using the KOCWIN v2.00 QSAR method (ECHA). Based on this K_{oc} value, if released to soil, magnesium silicate hydrate (talc) is expected to a low potential for adsorption. If released into water, the substance has a low potential for adsorption to sediment or suspended solids.

D. Bioaccumulation

There is no potential for bioaccumulation. Due to its inherent chemical-physical properties, such as absence of lipophilicity as well as the capability of the organism to excrete absorbed SiO_2 components, bioaccumulation can be disregarded. Magnesium is widespread in living cells and does not bioconcentrate in aquatic organisms (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Talc does not bioaccumulate, is not persistent and is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Table 3 lists the results of the acute aquatic toxicity studies on magnesium silicate hydrate (talc).
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Table 3 Acute Aquatic Toxicity Studies on Talc

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fish (species unnamed)	96-hr LC_{50}	89,581 mg/L (QSAR)	2	ECHA
Daphnid	48-hr LC_{50}	36,812 mg/L (QSAR)	2	ECHA
Algae (species unnamed)	96-hr LC_{50}	7,203 mg/L	1	ECHA

Chronic Studies

No data are available. Short term aquatic toxicity tests reported in the literature on fish (LC_{50} *Brachydanio rerio* (Zebra fish) >100000 mg/L/24 hr; for Talc) show this substance is not toxic to aquatic life. On this basis the need for long term aquatic testing is waived (ECHA).

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Magnesium silicate hydrate (talc) is an inorganic substance and thus, biodegradation is not relevant. For the purposes of this PBT assessment, the persistent criteria are not considered applicable for this substance.

No data are available on bioaccumulation. However, based on the low log K_{ow}, and the inherent chemical-physical properties of magnesium silicate hydrate (talc), bioaccumulation is not expected. Thus, magnesium silicate hydrate (talc) does not meet the screening criteria for bioaccumulation.

Chronic aquatic toxicity data is not available. The EC_{50} values from the acute aquatic toxicity studies on magnesium silicate hydrate (talc) are >1 mg/L. Thus, magnesium silicate hydrate (talc) does not meet the criteria for toxicity

Therefore, magnesium silicate hydrate (talc) is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for magnesium silicate hydrate (talc).

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Magnesium silicate hydrate (talc)	14807-96-6	Not a PBT	No	No	NA	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2017). Chemicals of low concern for human health based on an initial assessment of hazards, Project report prepared by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
KOCWIN	USEPA organic carbon partition coefficient estimation model
kg/m^3	kilogram per cubic metre

kPa	kilopascal
LC	lethal concentration
L/Kg	litres per kilogram
mg/L	milligrams per litre
NOEC	no observed effect concentration
Pa	Pascal
PBT	Persistent Bioaccumulative Toxic
QSAR	quantitative structure-activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

MELAMINE, FORMALDEHYDE, SODIUM BISULFITE POLYMER

This dossier on melamine, formaldehyde, sodium bisulfite polymer presents the most critical studies pertinent to the risk assessment of melamine, formaldehyde, sodium bisulfite polymer in its use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Melamine, formaldehyde, sodium bisulfite polymer is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Melamine, formaldehyde, sodium bisulfite polymer is used as a cement additive in the drilling process. As a polymer the substance is not expected to bioconcentrate, bioaccumulate or sorb substantially to soils or sediments. It is not expected to degrade in the environment. Furthermore, it is expected to be of relatively low toxicity to environmental receptors. Thus, the substance is considered a polymer of low concern by NICNAS in an IMAP Tier 1 assessment.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sulfurous acid, monosodium salt, polymer with formaldehyde and 1,3,5-triazine-2,4,6-triamine

CAS RN: 64787-97-9

Molecular formula: $(C_3H_6N_6.HC_2O.H_2O_3S.Na)_x$ [This substance is a polymer.]

Molecular weight: Unknown

Synonyms: Melamine, formaldehyde, sodium bisulfite polymer; sulfurous acid, monosodium salt, polymer with formaldehyde and 1,3,5-triazine-2,4,6-triamine; sulfurous acid, sodium salt (1:1), polymer with formaldehyde and 1,3,5-triazine-2,4,6-triamine

3 PHYSICO-CHEMICAL PROPERTIES

No information is available.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for melamine, formaldehyde, sodium bisulfite polymer.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No data are available.

6 ENVIRONMENTAL EFFECTS SUMMARY

NICNAS has assessed melamine, formaldehyde, sodium bisulfite polymer in an IMAP Tier 1 assessment and considers it a "polymer identified as a low concern to the environment."[1]. As a polymer of low concern, the substance is not expected to bioaccumulate or bioconcentrate. It may sorb to sediments and soil; however, it is not expected to exhibit toxicity to environmental receptors.

The Government of Canada reported an acute aquatic toxicity study[2] for a 96-hour LC_{50} in *Daphnia Magna* as >100 mg/L, further supporting low toxicity.

No other data was available.

A. Terrestrial Toxicity

No data are available.

[1] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.

[2] https://canadachemicals.oecd.org/ChemicalDetails.aspx?ChemicalID=DB0B6224-611B-43CE-8BBE-BCBC89FAF007

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Melamine, formaldehyde, sodium bisulfite polymer is not expected to be biodegradable. Thus, it meets the criteria for persistence.

Melamine, formaldehyde, sodium bisulfite polymer is not expected to bioaccumulate due to its low potential for bioavailability because of its expected molecular weight and size and low water solubility.

No aquatic toxicity studies are available for melamine, formaldehyde, sodium bisulfite polymer. It is expected to be a low concern of toxicity to aquatic organisms because of its low potential for bioavailability.

The overall conclusion is that melamine, formaldehyde, sodium bisulfite polymer is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for melamine, formaldehyde, sodium bisulfite polymer.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Melamine, formaldehyde, sodium bisulfite polymer	64787-97-9	Not a PBT	No	Yes	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IMAP	Inventory Multi-Tiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

METHANOL

This dossier on methanol presents the most critical studies pertinent to the risk assessment of methanol in its use in drilling muds and hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on methanol (OECD, 2004a,b), and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Methanol is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Methanol is a liquid at room temperature. It is readily bioavailable and will not bioaccumulate. Methanol exhibits a low toxicity concern for aquatic organisms, terrestrial invertebrates and plants.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Methanol

CAS RN: 67-56-1

Molecular formula: CH_4O

Molecular weight: 32.04 g/mol

Synonyms: Methyl alcohol, carbinol, wood spirits, wood alcohol, methylol, wood, columbian spirits, colonial spirit, columbian spirit, methyl hydroxide, monohydroxymethane, pyroxylic spirit, wood naphtha.

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Physico-Chemical Properties of Methanol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid	2	ECHA
Melting Point	-97.8°C @ 101.3 kPa	2	ECHA
Boiling Point	64.7°C @ 101.3 kPa	2	ECHA
Density	790 Kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	16927 Pa @ 25°C	2	ECHA
Partition Coefficient (log Pow)	-0.77 @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	>1,000 g/L [miscible]	2	ECHA
Viscosity	0.544 – 0.59 mPa s (dynamic)	2	ECHA

Methanol is a highly flammable liquid.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for methanol.

Based on an assessment of environmental hazards, NICNAS identified methanol as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Methanol is readily biodegradable. It has a low adsorptive capacity to soils and is unlikely to bioaccumulate.

B. Partitioning

Methanol is highly soluble in water. Based upon a Henry's Law constant of 0.461 Pa*m^3/mol, it is expected to volatilise from water and moist soil surfaces. It is also expected to volatilise from dry soil surfaces based upon its vapour pressure(PubChem). Vapour-phase methanol will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 17.2 days (ECHA).

C. Biodegradation

Methanol is readily biodegradable. In a closed bottle test using seawater, there was 84% and 95% degradation after 10 and 20 days, respectively (Price et al., 1974; ECHA). [Kl. score = 2]

In a soil test using [^{14}C]-methanol, there was 53.4% degradation under aerobic conditions after 5 days, as measured by CO_2 evolution; and 46.3% degradation under anaerobic conditions after 5 days, as measured by CO_2 evolution (Scheunert et al., 1987; ECHA). [Kl. score = 2]

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

The adsorption of methanol was investigated in three different soil types at 6°C (Lokke, 1984; ECHA). There was slight adsorption with the sandy soils tested (percentage organic matter of 0.09% and 0.1% in the samples) and with the clay soil (percentage organic matter was 0.22%). Methanol solutions of concentrations of 0.1, 1.0, 9 and 90 mg/L were used in one-hour exposure adsorption studies; the K_{oc} values were between 0.13 and 0.61 for all soil types and at all concentrations.

Based upon these K_{oc} values, if released to soil, methanol is expected to have very high mobility. If released into water, due to its high water solubility and low K_{oc}, methanol is not expected to adsorb to suspended solids and sediment in water.

E. Bioaccumulation

The BCF of methanol in *Cyprinus carpio* was determined to be 1.0 (Gluth et al. 1985); in *Leuciscus idus*, the BCF was <10 (Hansch and Leo, 1985; Freitag et al. 1985). Therefore, the potential for bioaccumulation is low.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Methanol exhibits a low toxicity concern for aquatic organisms, terrestrial invertebrates, and plants.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on methanol.

Table 3 Acute Aquatic Toxicity Studies on Methanol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Bluegill	96-hour LC_{50}	15,400	1	Poirer et al. 1986
Salmo gairdneri	96-hour LC_{50}	20,100	1	Call et al., 1983
Pimphales promelas	96-hour LC_{50}	28,100	1	Call et al., 1983

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	96-hour EC_{50}	18,260	2	Dorn et al., 2012; ECHA
Daphnia magna	48-hour EC_{50}	>10,000	2	Kuehn et al., 1989
Selenastrum capricornutum	96-hour EC_{50}	~22,000	2	Cho et al., 2008; ECHA
Chlorella pyrenoidosa	10-14 day EC_{50}	28,400	2	Stratton and Smith, 1988

Chronic Studies

No adequate chronic studies were identified. Reported studies were either invalid or their reliability was questionable. Methanol belongs to the category of organic chemicals exerting toxicity for aquatic organisms with a non-specific mode of action. The acute and chronic toxicity may be estimated for such kind of chemicals using QSAR methods. The ECOSAR model (version 1.11, US EPA, July 2012) predicts for methanol a chronic toxicity value of about 450 mg/L (equivalent to a NOEC) for *Pimephales promelas* and a value of 208 mg/L for *Daphnia magna* (REACH) [Kl. score = 1].

C. Terrestrial Toxicity

The terrestrial toxicity studies on methanol are listed below in Table 4.

Table 4 Terrestrial Toxicity Studies on Methanol

Test Species (Method)	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Earthworm *Eisenia fetida* (OECD 222)	35-d EC_{50} 63-d EC_{50}	17,199 26,646	2	ECHA
Folsomia candida (OECD 232)	28-d EC_{25} 28-d NOEC* (reproduction)	2,842 1,000	1	ECHA
Hordeum vulgare (OECD 208)	14-d EC_{50} 14-d NOEC* (seedling emergence)	15,492 12,000	1	ECHA
	14-d EC_{25} 14-d NOEC* (shoot dry mass)	2,538 1,555		
	14-d EC_{25} 14-d NOEC* (root dry mass)	2,823 2,592		
	14-d EC_{25} 14-d NOEC* (shoot length)	4,885 2,592		
	14-d EC_{25} 14-d NOEC* (root length)	5,752 4,320		

* Since only EC_{25} values were available from the test results, NOECs were derived graphically from the representing treatment means.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009, ECHA, 2008).

Methanol is readily biodegradable and thus it does not meet the screening criteria for persistence.

Based on an experimental BCF of <10 in fish, methanol does not meet the criteria for bioaccumulation.

There are no adequate chronic toxicity studies on methanol. Predicted toxicity based on QSAR methods indicates chronic values > 0.1 mg/L for fish and invertebrates. The acute EC_{50} values of methanol in fish, invertebrates and algae is >1 mg/L; thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that methanol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for methanol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Methanol	67-56-1	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
BCF	bioconcentration factor
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration

mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa m^3/mol	Pascal metre cubed per gram molecular weight
PBT	Persistent, Bioaccumulative and Toxic
QSAR	Quantitative structure-activity relationship
SIDS	Screening Information Data Set

METHYL ACETATE

This dossier on methyl acetate presents the most critical studies pertinent to the risk assessment of methyl acetate in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Methyl acetate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Methyl acetate is a carboxylate ester and is used as a solvent, being both weakly polar and lipophilic. The substance is readily biodegradable, is not expected to bioaccumulate and has a low tendency to bind to soil or sediment. Methyl acetate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): methyl acetate

CAS RN: 79-20-9

Molecular formula: $C_3H_6O_2$

Molecular weight: 74.08 g/mol

Synonyms: Methyl acetic ester, Ethyl ester of monoacetic acid, Methyl ethanoate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Methyl Acetate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	colourless organic liquid	2	ECHA
Melting Point	-98 °C @ 101.3 kPa	2	ECHA
Boiling Point	57 °C @ 101.3 kPa	2	ECHA
Density	930 kg/m^3 @ 20 °C	2	ECHA
Vapour Pressure	22,800 Pa @ 20 °C	2	ECHA
Partition Coefficient (log P_{ow})	0.18	2	ECHA
Water Solubility	243.5 g/L @ 20 °C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for methyl acetate.

NICNAS has assessed methyl acetate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Methyl acetate is readily biodegradable and is not expected to bioaccumulate. It has a low tendency to bind to soil or sediment.

B. Partitioning

Volatilisation of methyl acetate from water and moist soil surfaces is expected to be an important fate process given a Henry's Law constant of 6.43 Pa-m^3/mole (ECHA). Methyl acetate is also expected to volatilise from dry soil surfaces based upon its vapour pressure. (PubChem).

C. Biodegradation

Methyl acetate is readily biodegradable. Biodegradation was tested according to OECD 301 (301 C and 301 D) of which the test according to OECD 301 D over a period of 28 days is the most reliable. The mean degradation rate of methyl acetate based on oxygen was > 68% within the 10-day window and reached 70% at the end of the test period. (ECHA)[KI Score = 2]

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=79-20-9%2C+

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

The adsorption coefficient of methyl acetate was determined by HPLC method. The capacity factors k' were calculated. The log k' value were plotted against the respective log K_{oc} values of the reference substances. The log Koc value of methyl acetate was calculated by means of the regression line equation resulting in 0.18. (ECHA)[Kl Score = 2].

Based on this value, methyl acetate has a low potential for adsorption to soil and is expected to have very high mobility. If released to water, based on this value and its water solubility, it is also not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

No bioconcentration studies have been conducted on methyl acetate. Methyl acetate is not expected to bioaccumulate based on the low experimental log K_{ow} of 0.18 (ECHA) [Kl. Score = 1].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Methyl acetate is of low toxicity concern to aquatic organisms.

A. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on methyl acetate.

Table 3 Acute Aquatic Toxicity Studies on Methyl Acetate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachidanio rerio	96-hr LC_{50}	250 - 350 mg /L	2	ECHA
Pimephales promelas	96-hr LC_{50}	>100	2	ECHA
Daphnia magna	48-hr EC_{50}	1026.7	2	ECHA
Scenedesmus subspicatus.	72-hr EC_{50}	>120	2	ECHA

Chronic Studies

No chronic data are available.

B. Terrestrial Toxicity

No studies are available. Methyl acetate is not expected to cause toxicity to terrestrial organisms (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Methyl acetate is readily biodegradable and thus does not meet the screening criteria for persistence.

The experimental log K_{ow} for methyl acetate is 0.18. Thus, methyl acetate does not meet the criteria for bioaccumulation.

There are no chronic toxicity studies on methyl acetate. The acute EC_{50} values for methyl acetate across several species is >1 mg/L. Thus, methyl acetate does not meet the screening criteria for toxicity.

The overall conclusion is that methyl acetate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for methyl acetate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Methyl acetate	79-20-9	Not a PBT	No	No	No	No	No	No	1	No data available	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

MODIFIED BENTONITE
[QUATERNARY AMMONIUM COMPOUNDS, BENZYL(HYDROGENATED TALLOW ALKYL)DIMETHYL, CHLORIDES, COMPOUNDS WITH BENTONITE]

This dossier is for modified bentonite: quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite (CAS No. 71011-24-0). For the purposes of this dossier, this substance will be referred to as benzyl monoalkyl chain quaternary ammonium compound [B(Alk)2M] bentonite.

This dossier presents the most critical studies pertinent to the risk assessment of B(Alk)2M bentonite in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the OECD-SIDS Initial Assessment Profile on the Organoclays Category (OECD, 2007). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Modified bentonite is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

The organoclays discussed in this dossier are hydrogenated tallowalkonium bentonites, and are the product of the reaction of hydrogenated tallowalkonium chloride and bentonite. Bentonite is a widely distributed, natural material consisting predominantly of the clay montmorillonite, a smectite clay. B(Alk)2M bentonite is not hydrolysable; the organic component is expected to have some limited biodegradation based on structurally similar material. Bioaccumulation is not expected due to the insolubility nature of B(Alk)2M bentonite. B(Alk)2M bentonite is virtually non-toxic to terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite

CAS RN: 71011-24-0

Molecular formula: Unspecified

Molecular weight: Unspecified

Synonyms: Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite; dimethyl dibenzyl hydrogenated tallow ammonium chloride reaction product with bentonite; hydrogenated tallow alkyl dimethyl dibenzyl ammonium bentonite salts

3 PHYSICO-CHEMICAL PROPERTIES

Organoclays, such as B(Alk)2M bentonite, are free flowing solid powders that are essentially insoluble in water, in organic solvents and in lipids. They are not volatile under ambient conditions. The organoclays do not melt or boil, although some degradation may occur when subjected to extreme heat at about 180^0C to 600^oC. The densities range from 1.4 to 1.8 (OECD, 2007).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for modified bentonite.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

B(Alk)2M bentonite is not hydrolysable; the organic component is expected to have some limited biodegradation based on structurally similar material. Bioaccumulation is not expected due to the insolubile nature of B(Alk)2M bentonite. Quaternary ammonium ions are tightly held to the clay, resulting in organoclay compounds (“salts”) that are very hydrophobic in nature (OECD, 2007).

B. Partitioning

Organoclays will not hydrolyse; they are resistant to base or acid attack over a pH range of 3 to 11 (OECD, 2007).

C. Biodegradation

No studies are available on B(Alk)2M bentonite.

OECD TG 306 studies have been carried out on a structurally similar organoclay, B(2Alk)M hectorite. This substance is quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (CAS No. 121888-67-3). Depending on the test, degradation ranged from 4.7% to

33.4% after 28 days, indicating limited biodegradation but not ready biodegradation. The biodegradation only occurs to the organic component of the organoclay (OECD, 2007).

D. Environmental Distribution

Quaternary ammonium ions are tightly held to the clay, resulting in organoclay compounds ("salts") that are very hydrophobic in nature (OECD, 2007).

E. Bioaccumulation

Bioaccumulation is not expected due to the insolubility nature of B(Alk)2M bentonite.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

B(Alk)2M bentonite has low acute toxicity to fish and invertebrates, with likely low acute toxicity to algae. A chronic *Daphnia* study conducted on an organoclay similar to B(Alk)2M bentonite suggests that these compounds may have moderate chronic toxicity concerns for aquatic organisms. However, the toxicity observed in the study has been due, in part, to the physical effects of the organoclay test material. B(Alk)2M bentonite is virtually non-toxic to terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Table 2 lists the results of acute aquatic toxicity studies on B(Alk)2M bentonite and similar organoclays.

Table 2 Acute Aquatic Toxicity Studies on B(Alk)2M Bentonite and Similar Organoclays

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Rainbow trout	96-hour LC_{50}	> ca. 500	4	OECD, 2007
Daphnia magna	96-hour EC_{50}	300	4	OECD, 2007
Daphnia magna	48-hour EC_{50}	<500*	4	OECD, 2007
Skeletonema costatum	72-hour EC_{50}	23.8** (growth rate)	4	OECD, 2007
Skeletonema costatum	72-hour EC_{50}	82.3 (growth rate)	4	OECD, 2007
Skeletonema costatum	72-hour EC_{50}	>1,000** (growth rate)	4	OECD, 2007
Skeletonema costatum	72-hour EC_{50} NOEC	>100 (growth rate)*** 100	4	OECD, 2007

*Only one concentration was used.
**Test material was B(2Alk)M bentonite. This compound is quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, chlorides, compounds with bentonite (CAS No. 68153-30-0).
***Test material was B(2Alk)M hectorite (CAS No. 121888-67-3).

The low algal 72-hour EC_{50} value of 23.8 mg/L for B(2Alk)M may have been due to physical toxicity; however, the study report did not provide additional information regarding how the test material was dispensed.

Chronic Studies

No studies are available on B(Alk)2M bentonite. A study is available on B(2Alk)M hectorite (CAS No. 121888-67-3).

The 21-day NOEC in a *Daphnia* reproduction test on B(2Alk)M hectorite was 3.2 mg/L (OECD, 2007). The mortality of *Daphnia* seen at the LOEC of 32 mg/L was considered to be due, in part, to physical effects of the test material.

C. Terrestrial Toxicity

The 14-day NOEC of B(Alk)2M bentonite to earthworms is 1,000 mg/kg. Since 1,000 mg/kg is the limit dose, it is assumed that the LC_{50} is >1,000 mg/kg (OECD, 2007).

Terrestrial plant toxicity are available for B(2Alk)M hectorite (CAS No. 12188-67-3). The EC_{50} values of B(2Alk)M hectorite for the emergence and early growth stages of wheat and radish seedlings (*Tritium aestivum* and *Raphanus sativus*, respectively) are >100 mg/kg; the NOEC are 100 mg/kg, the highest dose tested (OECD, 2007). The LC_{50} of B(2Alk)M hectorite was 9 mg/kg for the emergence and early growth stages of cress seedling (*Lepidum sativum*); the LOEC was 1 mg/kg and a NOEC was not established (OECD, 2007).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The clay component of B(Alk)2M bentonite is not biodegradable, and the organic component is not readily biodegradable. Thus, it meets the criteria for persistence.

B(Alk)2M bentonite is insoluble in water and is not bioavailable. Thus, it is not expected to meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies available on B(Alk)2M bentonite; however, the NOEC from a chronic *Daphnia* study on a similar organoclay is >0.1 mg/L. The acute EC_{50} values for B(Alk)2M bentonite and similar organoclays are >1 mg/L in fish, invertebrates and algae. Thus, it does not meet the criteria for toxicity.

The overall conclusion is that B(Alk)2m bentonite is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for modified bentonite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Modified Bentonite	71011-24-0	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

OECD. (2007). SIDS Initial Assessment Profile on Organoclays Category. Available at: https://hpvchemicals.oecd.org/ui/handler.axd?id=b8b51b84-081c-444c-bb95-fb7f41c859c1

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
LC	lethal concentration
LOEC	lowest observed effective concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

TG test guideline

MONOETHANOLAMINE BORATE

This dossier on monoethanolamine borate presents the most critical studies pertinent to the risk assessment of monoethanolamine borate in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Monoethanolamine borate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Monoethanolamine borate is readily biodegradable. It will not adsorb significantly to suspended solids and sediments in water and would be highly mobile in soil. It has a low potential for bioaccumulation. Monoethanolamine borate has a moderate acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Reaction products of monoethanolamine and boric acid (1:3)

CAS RN: 26038-87-9

Molecular formula: $C_2H_7NO.xBH_3O_3$ [UVCB substance]

Molecular weight: 166.97 g/mol

Synonyms: Monoethanolamine borate; orthoboric acid, compound with 2-aminoethanol; boric acid (H_3BO_3), reaction products with ethanolamine; MEA polyborate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Monoethanolamine Borate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	2	ECHA
Melting Point	NA	-	ECHA
Boiling Point	NA	-	ECHA
Density	≤1245 Kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	<0 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	-0.9 (polyborate moiety) @ 19.7 °C	1	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	1.47 g/L @ 20°C	1	ECHA

Monoethanolamine borate only exists in aqueous solution. It exists in a constant state of equilibrium, and attempts to remove the water result in a shift of equilibrium, and a change in the nature of the molecule (ECHA).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for monoethanolamine borate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Monoethanolamine borate is readily biodegradable. It will not adsorb significantly to suspended solids and sediments in water and would be highly mobile in soil. It has a low potential for bioaccumulation.

B. Partitioning

Monoethanolamine borate is infinitely soluble in water. Chemicals in this group will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions (NICNAS, 2019).

C. Biodegradation

Monoethanolamine borate 1:1 is readily biodegradable. In a modified Sturm test (OECD 301B), degradation was 73% after 28 days; the 10-day window was met (ECHA). [Kl. score = 1]

Monoethanolamine borate 1:3 is readily biodegradable. In a modified Sturm test (OECD 301B), degradation was 75% after 28 days; the 10-day window was met (ECHA).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

The log K_{oc} was determined for monoethanolamine borate 1:1 and monoethanolamine borate 1:3 on soil and on sewage sludge using high performance liquid chromatography (HPLC). Both the monoethanolamine and the polyborate part of both substances did not significantly adsorb to soil. The experimental log K_{oc} was determined to be approximately 1.26 [K_{oc} = 18.2 L/kg] (ECHA). [Kl. score = 1] Based on this low K_{oc} value and infinite water solubility, this substance in highly mobile in soil.

E. Bioaccumulation

No bioconcentration studies are available. In an OECD 107 study, the log K_{ow} was determined to be -0.9 for the polyborate moiety and -2.5 for the organic moiety. Based on a log K_{ow} of < 3, this substance has a low potential for bioaccumulation (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Monoethanolamine borate has moderate acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on monoethanolamine borate.

Table 3 Acute Aquatic Toxicity Studies on Monoethanolamine Borate

Test Species	Test Substance	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rario	Monoethanol-amine borate 1:1	96-hour LC_{50}	>100	1	ECHA
Carp	Monoethanol-amine borate 1:3	96-hour LC_{50}	617	1	ECHA
Daphnia magna	Monoethanol-amine borate 1:3	48-hour EC_{50}	496	1	ECHA
Daphnia magna	Monoethanol-amine borate 1:1	48-hour EC_{50}	423	1	ECHA
Pseudokirchneriella subcapitata	Monoethanol-amine borate 1:3	72-hour EC_{50} NOEC	67 (growth rate) 72 (biomass) 18 (growth rate)	1	ECHA

Test Species	Test Substance	Endpoint	Results (mg/L)	Klimisch score	Reference
Pseudokirchneriella subcapitata	Monoethanol-amine borate 1:1	72-hour EC_{50}	26 (growth rate) 13 (biomass) 3.2 (growth rate)	1	ECHA

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Monoethanolamine borate is readily biodegradable; thus it does not meet the screening criteria for persistence.

No bioconcentration studies have been conducted on monoethanolamine borate. The log K_{ow} is <3. Thus, acetic acid does not meet the screening criteria for bioaccumulation.

No chronic aquatic toxicity studies are available for monoethanolamine borate. The acute EC_{50} values in fish, invertebrates and algae are >1 mg/L. Thus monoethanolamine borate does not meet the criteria for toxicity.

The overall conclusion is that monoethanolamine borate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for monoethanolamine borate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Monoethanolamine Borate	26038-87-9	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2019). Boric acid and precursors to boric acid: Environment tier II assessment. Available on-line: https://www.industrialchemicals.gov.au/sites/default/files/Boric%20acid%20and%20precursors%20to%20boric%20acid_%20Environment%20tier%20II%20assessment.pdf

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HPLC	high performance liquid chromatography
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal

L/kg	litres per kilogram
LC	lethal concentration
MEA	monoethanolamine
mg/L	milligrams per litre
NA	not applicable
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

NITRILOTRIACETIC ACID, TRISODIUM SALT MONOHYDRATE

This dossier on nitrilotriacetic acid, trisodium salt monohydrate presents the most critical studies pertinent to the risk assessment of nitrilotriacetic acid, trisodium salt monohydrate in its use in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Nitrilotriacetic acid, trisodium salt monohydrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Nitrilotriacetic acid, trisodium salt monohydrate (Na_3NTA) is an organic sodium salt composed of sodium and nitrilotriacetate ions in a 3:1 ratio. Na_3NTA dissociate to form a common moiety, nitrilotriacetate ion. The substance is used to soften water and to remove traces of heavy metals. It is also commonly used as chelating and sequestering agents, and as builders in detergent and cleaning formulations for domestic and commercial use.

Na_3NTA is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil. It exhibits low toxicity to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): trisodium-2-[bis(carboxymethyl)amino]acetate

CAS RN: 5064-31-3

Molecular formula: $C_6H_9NO_6.3Na$

Molecular weight: 257.08 g/mol

Synonyms: Trisodium nitrilotriacetate; glycine, N,N-bis(carboxymethyl)-,trisodium salt; trisodium 2,2’,2”-nitrilotriacetate; Nitrilo triacetic acid, trisodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Na_3NTA

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	2	ECHA
Melting Point	340°C (decomposes) (pressure not provided)	2	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	No data as the substance is a solid which melts above 300°C	-	ECHA
Density	1770 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	-	-	ECHA
Partition Coefficient (log K_{ow})	-13.2 @ 25°C	2	ECHA
Water Solubility	457 g/L @ 20°C	2	ECHA
Viscosity	Not applicable	-	ECHA
Dissociation constant	1.22 @ 25°C	2	ECHA

Since sodium salts are generally considered to be completely dissociating, a solution of Na_3NTA in water yields the tribasic anion nitrilotriacetate. Na_3NTA is a weak acid, and in such a solution, the NTA will therefore exist as an equilibrium mixture of several species:

$NTA^{---} <-> HNTA^{--} <-> H_2NTA^{-} <-> H_3NTA <-> H_4NTA^{+}$

with the last species occurring when, in a very acidic environment, the central nitrogen atom is protonated (ECHA).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for nitrilotriacetic acid, trisodium salt monohydrate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Na_3NTA is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Biodegradation

Na_3NTA was tested for ready biodegradability according to OECD 301 E (BASF, 1983b,c), OECD 301 F (in addition to a combined CO2/DOC test, see Strotmann et al., 1995), and Sturm Test (BASF, 1983d), and in a die away test (Takahashi et al, 1997) as well as for inherent biodegradability according to OECD 302 B (BASF, 1983a). These tests resulted in 75 -100 % degradation after 7 to 28 days with lag phases ranging between 1 and 16 days. According to results from ready biodegradation tests, Na3NTA can be regarded as readily biodegradable (ECHA) [Kl. Score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

A relevant adsorption of Na_3NTA onto the organic fraction of soils, sediments or suspended solids is not expected due to the ionic structure of the substance and a log K_{ow} of -13.2 (pH 7). However, interaction with the mineral phase may be possible (ECHA) [Kl. Score = 2]. Based on its low log K_{ow} and high water solubility values, if released to soil, Na_3NTA is expected to have low potential for adsorption and a high potential for mobility. If released to water, it is likely to remain in water and not adsorb to sediment.

D. Bioaccumulation

There are no bioaccumulation studies on Na_3NTA. Bioaccumulation of Na_3NTA is not expected to occur because of its log K_{ow} of -13.2 at pH 7, is highly water-soluble, and is unlikely, due to its polar nature, to be taken up by fish gills or across other biological membranes (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Na_3NTA exhibits low toxicity to aquatic and terrestrial organisms. Details are provided below.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 presents the results of acute aquatic toxicity studies on Na_3NTA.

Table 3 Acute Aquatic Toxicity Studies on Na_3NTA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	103	2	ECHA
Gammarus pseudolimnaeus	96-hour LC_{50}	80	2	ECHA
Scenedesmus subspicatus	72-hour EC_{50}	>91.5	1	ECHA

Other data were deemed as less reliable; and, as a result, are not shown in Table 3.

Chronic Studies

In a 32-week fish (*Pimephales promelas*) chronic study, the measured NOEC values>= 54 mg/L (ECHA). [Kl. score = 2]. In a 27-day fish (Oncorhyncus mykiss) chronic study, the measured LC_{50} value for 50 mg/L hardness was 90.5 mg/L and for 200 mg/L hardness was 114 mg/L (ECHA) [Kl. Score = 2].

In a 21-week *Gammarus psuedolimnaeus* reproduction study, the measured NOEC value was 9.3 mg/L (ECHA). [Kl. score = 2].

In a 21-day *Daphnia* reproduction study, the measured NOEC value was 100 mg/L for survival and reproduction (ECHA). [Kl. score = 3]

In a 120-day *Helisoma trivolvis* reproduction study, the measured NOEC value was 12.5 mg/L for growth (ECHA) [Kl. Score = 2].

C. Terrestrial Toxicity

There are no ecotoxicity studies for terrestrial organisms relating to Na_3NTA. It is reasonable to assume that trends seen in aquatic toxicity are likely to be observed in terrestrial organisms. These short- and long-term aquatic data, when considered with bioaccumulative and degradation information, result in Na_3NTA being practically non-toxic to aquatic organisms. It is reasonable to assume that Na_3NTA will also be non-toxic to soil organisms (ECHA).

7 CATEGORISATION AND OTHER CHARCTERSTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Na_3NTA is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -13.2, Na_3NTA does not meet the screening criteria for bioaccumulation.

The lowest chronic EC_{10} or NOEC value for Na_3NTA is >0.1 mg/L. The acute EC_{50} values are >1 mg/L. Thus, Na_3NTA does not meet the criteria for toxicity.

The overall conclusion is that Na_3NTA is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for Na_3NTA.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Nitrilotriacetic acid, trisodium salt monohydrate	5064-31-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model

kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

NITROGEN

This dossier on nitrogen presents the most critical studies pertinent to the risk assessment of nitrogen in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Nitrogen is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Nitrogen (or nitrogen gas) is an inert diatomic gas that comprises 76% of air by mass. Nitrogen gas is separated from the atmosphere on an industrial scale and is used as an inert gas or foaming agent in a wide range of industries. It is reported to be used in the Australian coal seam gas industry within hydraulic fracturing or pre-treatment formulations. Although its function was not specified, internationally this gas is known to be used for fracturing shallow and water sensitive formations that remain self-propped after fracturing. Additionally, nitrogen gas can be used as a fluid weight reducer and for proppant suspension in fracturing fluids (DoEE, 2017a).

Life is naturally adapted to high concentrations of nitrogen gas in the atmosphere and the presence of saturation concentrations of dinitrogen in water. Except for asphyxiation hazards associated with exclusion of oxygen by this inert gas, nitrogen gas is not considered to be hazardous to life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Nitrogen

CAS RN: 7727-37-9

Molecular formula: N_2

Molecular weight: 28.014 g/mol

Synonyms: Nitrogen gas; Dinitrogen

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Nitrogen

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	gas	-	PubChem
Melting Point	−210 °C (Pressure not provided)	-	PubChem

Property	Value	Klimisch score	Reference
Boiling Point	−195.79 °C (Pressure not provided)	-	PubChem
Partition Coefficient (log K_{ow})	0.67	-	PubChem
Density	1.2506 kg/m^3 @ 0 °C	-	PubChem
Water Solubility	18.1 g/L @ 21 °C	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for nitrogen.

Based on an assessment of hazards, NICNAS identified the substance as a chemical of low concern to human health and the environment (NICNAS, 2017 and DoEE, 2017b). Chemicals of low concern are considered to have a low likelihood of causing adverse human health effects should an exposure occur and are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Dinitrogen is an inert gas under normal atmospheric conditions and therefore has a natural tendency to partition and disperse into the air compartment. The very high measured Henry's Law constant (H = 153,846 Pa m^3 /mol) indicates that dissolved dinitrogen will partition overwhelming from water or moist soil into the air compartment, where nitrogen gas is the major constituent of the atmosphere (DoEE, 2017a).

Concentrations of dinitrogen in environmental waters are generally in equilibrium with the atmosphere. However, stratification effects and seasonal changes in dinitrogen consumption and production by the nitrogen cycle in natural water bodies can perturb local dissolved dinitrogen concentrations (Wetzel, 2001).

6 ENVIRONMENTAL EFFECTS SUMMARY

Nitrogen gas is the dominant constituent of the atmosphere and is also present at or near saturation concentrations in water. Life is naturally adapted to high concentrations of nitrogen gas in the atmosphere and the presence of saturation concentrations of dinitrogen in water. Except for asphyxiation hazards associated with exclusion of oxygen by this inert gas, nitrogen gas is not considered to be hazardous to life (DoEE, 2017a).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The biodegradation endpoint is not relevant for nitrogen. As such nitrogen does not meet the screening criteria for persistence.

Bioconcentration studies are not relevant for nitrogen. Therefore, nitrogen does not meet the screening criteria for bioaccumulation.

Nitrogen gas is the major constituent of the atmosphere. It is an inert non-toxic gas that is ubiquitous in the environment (DoEE, 2017a). Nitrogen does not meet the screening criteria for toxicity.

The overall conclusion is that nitrogen is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for nitrogen.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Nitrogen	7727-37-9	Not a PBT	No	No	NA	No	No	No	NA	NA	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy (DoEE). 2017b. Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

DoEE. 2017a. Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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Wetzel, RG. 2001. Limnology: lake and river ecosystems (3rd edition), Elsevier, San Diego.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts

EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

N,N-DIMETHYLMETHANAMINE

This dossier on N,N-dimethylmethanamine (trimethylamine) presents the most critical studies pertinent to the risk assessment of N,N-dimethylmethanamine in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – N,N-dimethylmethanamine (trimethylamine) is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

N,N-dimethylmethanamine is readily biodegradable. It unlikely to bioaccumulate; and it will not adsorb significantly to suspended solids and sediments in water and is highly mobile in soil. N,N-dimethylmethanamine has low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): trimethylamine

CAS RN: 75-50-3

Molecular formula: C_3H_9N or $(CH_3)_3N$

Molecular weight: 59.11 g/mol

Synonyms: N,N-dimethylmethanamine; trimethylamine; methanamine, N,N-dimethyl- (9CI); N-trimethylamine

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of N,N-dimethylmethanamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquified gas @ 20°C, with a pungent, fish ammonia-like odour	1	ECHA
Melting Point	-117.3°C to -117°C	2	ECHA
Boiling Point	2.9 to 3.5°C @ 101.3 kPa	2	ECHA
Density	630 to 670 kg/m^3 @ 20 °C	2	ECHA
Vapour Pressure	190900 Pa @ 20°C 214600 Pa @ 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	0.245 (pH 10 @ 25°C) <-3.5 (pH 7 with HCl @ 25°C)	2	ECHA
Water Solubility	409 g/L @ 19 °C	2	ECHA
Dissociation Constant (pKa)	9.8 @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for N,N-dimethylmethanamine.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

N,N-dimethylmethanamine is readily biodegradable. It unlikely to bioaccumulate; and it will not adsorb significantly to suspended solids and sediments in water and is highly mobile in soil.

B. Partitioning

N,N-dimethylmethanamine is highly soluble in water. Based on its Henry's Law Constant volatilisation from water or moist soil surfaces is not expected to be an important fate process. It is expected to volatilize from dry soil surfaces based upon its vapour pressure.

C. Biodegradation

N,N-dimethylmethanamine is readily biodegradable. In a OECD 301 C test, degradation was 92% in 14 days (ECHA). [Kl. score = 2]

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for N,N-dimethylmethanamine. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 8.876 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 7.32 L/kg.

If released to soil, based on this estimated Koc value, N,N-dimethylmethanamine is expected to have very high mobility. The pKa of trimethylamine is 9.8 (PubChem), indicating that this compound will exist almost entirely in the cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. If released into water, N,N-dimethylmethanamine is also not expected to adsorb to suspended solids and sediment based upon the estimated Koc and its high solubility.

E. Bioaccumulation

No bioconcentration studies have been conducted on N,N-dimethylmethanamine. N,N-dimethylmethanamine is not expected to bioaccumulate based on the experimental log K_{ow} of <-3.5 at pH 7 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

N,N-dimethylmethanamine has low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on N,N-dimethylmethanamine.

Table 3 Acute Aquatic Toxicity Studies on N,N-dimethylmethanamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Leuciscus idus	48-hr LC_{50}	25 (un-neutralised) 610 (neutralised)	2	ECHA
Daphnia magna	48-hr EC_{50}	139.95	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50} EC_{10}	150 (growth rate) 90.6 (biomass) 86 (growth rate) 42.6 (biomass)	2	ECHA

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies on N,N-dimethylmethanamine.

Table 4 Chronic Aquatic Toxicity Studies on N,N-dimethylmethanamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	EC_{10}	3.9	2	ECHA

No chronic studies were available for fish or algae.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

N,N-dimethylmethanamine is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of <-3.5 at pH 7, N,N-dimethylmethanamine does not meet the screening criteria for bioaccumulation.

The EC_{10} values from the chronic aquatic toxicity studies on N,N-dimethylmethanamine are >0.1 mg/L for invertebrates. There are no chronic toxicity studies on N,N-dimethylmethanamine for fish or algae. The acute $E(L)C_{50}$ values of N,N-dimethylmethanamine are >1 mg/L for fish, invertebrates and algae. Thus N,N-dimethylmethanamine does not meet the screening criteria for toxicity.

The overall conclusion is that N,N-dimethylmethanamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for N,N-dimethylmethanamine.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
N,N-dimethylmethanamine	75-50-3	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
atm m^3/mol	Atmosphere cubic meter per mol
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal

IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
kg/m^3	kilogram per cubic metre
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

POLYALKYLENE
[Polyalkylene Glycol Monobutyl Ether]

This dossier on polyalkylene or more specifically, polyalkylene glycol monobutyl ether, presents the most critical studies pertinent to the risk assessment of polyalkylene glycol monobutyl ether in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al*., 1997).

Screening Assessment Conclusion – Polyalkylene is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Polyalkylene is polyalkylene glycol monobutyl ether (PGME) polymers that vary in molecular weight (size). High molecular weight synthetic non-ionic polymers of this type are generally considered to be of low concern to the environment (Beothling and Nabholz 1997). They are not bioaccumulative and have low direct toxicity to aquatic organisms. Depending on the molecular weight, the degree of biodegradability can vary from slowly biodegradable (higher molecular weight) to readily biodegradable (lower molecular weight), although they generally have low mobility and very low bioavailability. Polyalkylene is practically non-toxic to aquatic organisms on an acute basis.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): butan-1-ol;ethane-1,2-diol;propane-1,2-diol

CAS RN: 9038-95-3

Molecular formula: $C_4H_{10}O.(C_3H_6O.C_2H_4O)_x$-

Molecular weight: variable

Synonyms: Methyloxirane polymer with oxirane monobutyl ester; methyloxirane, polymer with oxirane, monobutyl ether; propylene oxide ethylene oxide polymer, monobutyl ether; polyalkylene glycol monobutyl ether; Tergitol nonionic XD; Tergitol XD (nonionic); Ucon 50-HB-2000; Ucon 50-HV-260; Ucon 50-HB-5100, Ucon fluid LB-285

3 PHYSICO-CHEMICAL PROPERTIES

High molecular weight (>1500) polyalkylene glycol monobutyl ether (PGME) polymers are colorless to yellow liquids with a mild odor and low volatility (do not evaporate easily at room temperature). Individual products vary in their average molecular weight and viscosity. Depending on the product's molecular weight, they are water-soluble at temperatures below 51-60°C (123.8-140°F), but completely insoluble at higher temperatures. PGME polymers do not readily lose their viscosity (shear stable), do not hydrolyze in the presence of acid, neutral, or base solutions. They show good oxidation resistance up to 500°F; are non-corrosive to common metals, have little or no effect on most rubber compounds and are miscible in hydrocarbon oils (USDA, 2013).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for polyalkylene.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No studies are available.

The following information is from the Dow Chemical Company's Product Safety Assessment document on their lower molecular weight polyalkylene glycol monobutyl ether (CAS RN 9038-95-3) branded products (Dow, 2014):

> SYNALOX and UCON Butanol-Propylene Oxide-Ethylene Oxide Based Polyglycols are nonvolatile (do not readily evaporate). These products have varying degrees of water solubility, from partial soluble to 100% miscible. If released to the environment, they would migrate toward or remain in water and adsorb on soil, sediment, and suspended solids. These products have varying degrees of biodegradability, from slowly biodegradable to readily biodegradable. For the slowly biodegradable products in this family, they would likely degrade slowly in the environment, including degradation by physical action or upon exposure to sunlight. For the products that are readily biodegradable, they would be rapidly biodegradable in various environmental media. These products are expected to be removed by waste-treatment facilities by adsorption to biosolids or biodegradation. Because of their relatively high molecular weight, and/or high water solubility, SYNALOX and UCON Butanol-Propylene Oxide-Ethylene Oxide Based Polyglycols are not likely to accumulate in the food chain (bioconcentration is low)".

The following information is from the Dow Chemical Company's Product Safety Assessment document on their high molecular weight polyalkylene glycol monobutyl ether (CASRN 9038-95-3) branded products (Dow, 2015).

> UCON™ 50-HB lubricants have low volatility (do not evaporate easily). Because they are water-soluble at room temperature, these lubricants will have the tendency to remain in

water with minimal tendency to bind to soil or sediment. UCON™ 50-HB lubricants are unlikely to persist in the environment. These compounds are moderately biodegradable which suggests they will be removed from water and soil environments, including biological wastewater treatment plants. UCON™ 50-HB lubricants are not likely to accumulate in the food chain (their bioconcentration potential is low).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No studies are available. These products are practically non-toxic (EC_{50}/LC_{50} >100 mg/L in the most sensitive species tested) to aquatic organisms on an acute basis.

B. Aquatic Toxicity

Acute Studies

No studies are available. The following information is from the Dow Chemical Company's Product Safety Assessment document on their low molecular weight polyalkylene glycol monobutyl ether (CAS RN 9038-95-3) branded products (Dow, 2014); it also applies to their high molecular weight branded products (Dow, 2015):

> [Polyalkylene glycol monobutyl ethers] are practically non-toxic to aquatic organisms (LC_{50}/EC_{50} >100 mg/L for the most sensitive species tested) on an acute basis.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The polyalkylene glycol monobutyl ethers can range from readily biodegradable to slowly biodegradable; thus, some of the polymers will not meet the screening criteria for persistence.

The polyalkylene glycol monobutyl ethers are expected to have high molecular weights and are not expected to be bioavailable. Thus, these polymers do not meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on the polyalkylene glycol monobutyl ethers. However, the acute EC_{50} on these polymers are >0.1 mg/L in aquatic organisms based on Dow Chemical's Product Safety Assessment (Dow, 2014 and 2015). The polyalkylene glycol monobutyl ethers also have a high molecular weight and are not expected to be bioavailable. Thus, they do not meet the screening criteria for toxicity.

The overall conclusion is that polyalkylene glycol monobutyl ethers are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for polyalkylene glycol monobutyl ether.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Polyalkylene Glycol Monobutyl Ether	9038-95-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).
3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Boethling, R.S. and Nabholz, J.V. (1997). 'Environmental assessment of polymers under the US Toxic Substances Control Act', in Hamilton J and Sutcliffe R (eds), Ecological assessment of polymers: strategies for product stewardship and regulatory programs, Van Nostrand Reinhold, New York, USA, pp 187-234.

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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Dow. (2015). UCON™ Lubricants (High Molecular Weight) UCON™ Lubricants 50-HB-2000, -3520, -5100, revised December 17, 2015.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

United States Department of Agriculture (USDA). 2013. Technical Evaluation Report: Polyalkylene glycol monobutyl ether (PGME) Handling/Processing. June 7, 2013.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
LC	lethal concentration
mg/L	milligrams per litre
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Polypropylene Glycol (CAS No. 25322-69-4)
Polypropylene (CAS No. 9003-07-0)

This dossier on polypropylene glycol (PPG) and similar polymer polypropylene presents the most critical studies pertinent to the risk assessment of these chemicals in their use in drilling muds. Information provided within this dossier is based primarily on PPG.

This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Polypropylene glycol and polypropylene are classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Polypropylene glycol or polypropylene oxide is the polymer of propylene glycol. Chemically it is a polyether, and, more generally speaking, it's a polyalkylene glycol. PPG is a liquid at room temperature. Solubility in water decreases rapidly with increasing molar mass. PPG is less toxic than polyethylene glycol (PEG) so biotechnologicals are now produced in PPG.

PPG is an organic substance that biodegrades readily, is not expected to bioaccumulate and has a low potential to adsorb to soil. PPG is of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-(2-hydroxypropoxy)propan-1-ol

CAS RN: 25322-69-4

Molecular formula: $C_6H_{14}O_3$

Molecular weight: 134.17 g/mol

Synonyms: 2-(2-hydroxypropoxy)propan-1-ol, Polypropylene glycol, 2-(2-hydroxypropoxy)-1-propanol, polyoxypropylene glycol, methyloxirane homopolymer, polyoxypropylene

Chemical Name (IUPAC): 12-[(2S,3R)-3-octyloxiran-2-yl]dodecanoic acid

CAS RN: 9003-07-0

Molecular formula: $(C_3H_6)_n$ (monomer); $C_{22}H_{42}O_3$ (polymer)

Molecular weight: 354.6 g/mol (polymer)

Synonyms: Polypropylene; 1-propene,homopolymer; propene polymers

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Polypropylene Glycol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Viscous colourless liquid	1	ECHA
Melting Point	No freezing down to -150°C	1	ECHA
Boiling Point	287.6°C @101.3 kPa	1	ECHA
Density	1012 kg/m^3@ 20°C	1	ECHA
Vapour Pressure	0.0839 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	0.01 @ 25°C	1	ECHA
Water Solubility	47 g/L at 22°C	1	ECHA
Viscosity	78.34 mPa s @20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for polypropylene glycol.

NICNAS has assessed PPG in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1].Likewise, NICNAS has assessed polypropylene as a low concern polymer for the environment and, similar to PPG, it poses no unreasonable risk to human health.[2]

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=25322-69-4%2C+

[2] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9003-07-0%2C+

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

PPG is an organic substance that biodegrades readily, is not expected to bioaccumulate and has a low potential to adsorb to soil.

B. Biodegradation

PPG has been determined to be readily biodegradable via an OECD Guideline 301 F test. After 28 days, 86.6% of the test substance had been degraded in a manometric respirometry test (ECHA) [Kl Score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental adsorption/desorption data are available for PPG. However, the estimated K_{oc} values for homologous components of this UVCB substance range from 1 to 10 L/kg for the lowest (least sorptive) and highest (most sorptive) molecular weight homologues. The components of this UVCB substance can be regarded as having low affinity for adsorption to soils and activated sludge biosolids (ECHA).

D. Bioaccumulation

Based on a log K_{ow} of <=3 and relatively high water solubility, PPG is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

PPG is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 presents the results of acute aquatic toxicity studies on PPG.

Table 3 Acute Aquatic Toxicity Studies on PPG

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hour LC_{50}	>100	2	ECHA
Daphnia magna	96-hour EC_{50}	105.8	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	>100	2	ECHA

Chronic Studies

No studies are available for PPG. Chronic toxicity to invertebrates of the structurally related substance D-Glucitol (Sorbitol), propoxylated (CAS# 52625-13-5) has been investigated in a reproduction test with Daphnia magna following the OECD guideline 211 using semi-static exposure. No effects were observed at the maximum concentration test (10 mg/l) and the NOEC are reported at 10 mg/l (nominal) for reproduction and mortality (ECHA) [Kl. Score = 1].

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

PPG is readily biodegradable; thus it does not meet the screening criteria for persistence.

No data are available on bioaccumulation. However, based on the low log K_{ow}, and rapid degradation rate, and significant water solubility, bioaccumulation is not expected.

No chronic toxicity studies are available for PPG. The NOEC values for a structurally related substance [D-Glucitol (Sorbitol), propoxylated (CAS# 52625-13-5)] are >0.1 mg/L for invertebrates. The acute E(L)C_{50} values of PPG are >1 mg/L for fish, invertebrates and algae. Thus, PPG does not meet the criteria for toxicity.

PPG is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for polypropylene glycol.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Polypropylene glycol	25322-69-4	Not a PBT	No	No	No	No	No	No	1	1	1
Polypropylene	9003-07-0	Not a PBT	No	Yes	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Pubchem. Open chemistry database at the National Institutes of Health (NIH). https://pubchem.ncbi.nlm.nih.gov/

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration

mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
PEG	polyethylene glycol
PPG	polypropylene glycol
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

POLYURETHANE FOAM

This dossier on polyurethane foam presents the most critical studies pertinent to the risk assessment of this polymer in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – polyurethane foam is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Polyurethane is a diverse group of polymers. The polymer with urethane can be used as a flexible or rigid foam, elastomer, coating, or adhesive. They can be made as thermoset and thermoplastic (Optinova, 2022). Thermoplastic polyurethane resin is used as a lost circulation material in drilling fluids.

Polyurethane foam is considered a generally inert chemical that is stable in the environment. Polyurethane is insoluble in water and synthetic polymers, such as polyurethane, by their nature are generally not considered to be biodegradable. Likewise, their physical size and resistance to biodegradation limits their bioavailability (Boethling and Nabholz, 1997). As a result, polyurethane is not expected to be harmful to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Ethyl Urea

CAS RN:9009-54-5

Molecular formula: $C_3H_8N_2O$

Molecular weight: 88.11 g/mol (monomer)

Synonyms: polyurethane; polyurethane (foam); aromatic type thermoplastic polyurethane resin; n-ethylurea; 1-ethylurea

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Polyurethane[1]

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Black or grey fine-sized reticulated foam, smaller than 7 mm	-	Halliburton, 2022
Melting Point	92.5°C (pressure not indicated)	-	PubChem
Boiling Point	206 °C (pressure not indicated)	-	USEPA, 2022
Density	1030 kg/m^3 (temperature not provided)	-	USEPA, 2022
Vapour Pressure	340 Pa @ 25 °C	-	USEPA, 2022
Partition Coefficient (log K_{ow})	-0.74	-	PubChem
Water Solubility	Insoluble in water (26 g/L @ 25 °C)	-	NLM, 2022

1 – Data provided for CAS No. 625-52-5 or 9009-54-5

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory) under alternate CAS No. 625-52-5. No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for polyurethane foam.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Polyurethane foam is considered a generally inert chemical that is stable in the environment. Polyurethane is insoluble in water and synthetic polymers, such as polyurethane, by their nature are generally not considered to be biodegradable. Likewise, their physical size and resistance to biodegradation limits their bioavailability (Boethling and Nabholz, 1997).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Polyurethane is expected to be of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

Limited ecotoxicity data is available for polyurethane. In 1999, USEPA conducted a validation study to evaluate Structure Activity Relationship (SAR) methods used to predict aquatic toxicity of polymers. The experimental data were obtained from an algae growth inhibition test, a Daphnia acute immobilisation test, or an acute toxicity test to Rainbow trout (*Oncorhychus mykiss*). The studies were conducted by four different contract laboratories located in the United States or in the United Kingdom following OECD guidelines and Good Laboratory Practice standards. For the polyurethanes tested, no acute toxicity (>100 mg/L) was observed for algae and invertebrates. Fish were not tested (USEPA, 2002).

Chronic Studies

There are no chronic studies available for polyurethane foam.

C. Terrestrial Toxicity

There are no studies available for polyurethane foam.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Polyurethane foam is considered not readily biodegradable; thus, it meets the screening criteria for persistence.

Polyurethane foam is expected to have a high molecular weight and poor water solubility. It is not expected to be bioavailable. Thus, this polymer does not meet the criteria for bioaccumulation.

There are no aquatic toxicity studies on polyurethane foam. However, no acute toxicity was observed in algae and invertebrates for other polyurethanes tested. Thus, polyurethane foam does not meet the screening criteria for toxicity.

The overall conclusion is that polyurethane foam is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for polyurethane foam.

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8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Polyurethane foam	9009-54-5	Not a PBT	No	No	Yes	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SDS	Safety Data Sheet
SGG	Synthetic Greenhouse Gases

POLY(VINYL ACETATE) – POLY(VINYL ALCOHOL) POLYMER

This dossier on poly(vinyl acetate)-poly(vinyl alcohol) polymer presents the most critical studies pertinent to the risk assessment of the substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Poly(vinyl acetate)-poly(vinyl alcohol) polymer is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Poly(vinyl acetate)-poly(vinyl alcohol) polymer is a vinyl polymer. Based largely on its high molecular weight, the substance is not expected to bioaccumulate or bioconcentrate. It is of low toxicity to environmental receptors and is not expected to degrade substantially under environmental conditions.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): ethenol; ethenyl acetate

CAS RN: 25213-24-5

Molecular formula: $(C_4H_6O_2.C_2H_4O)x$-[This substance is a polymer.]

Molecular weight: 130.1418 g/mol (monomer); polymer variable (UVCB)

Synonyms: Poly(vinyl acetate)-poly(vinyl alcohol) polymer; vinyl alcohol, polymer with vinyl acetate; ethanol-vinyl acetate copolymer; acetic acid ethenyl ester, polymer with ethenol

3 PHYSICO-CHEMICAL PROPERTIES

No chemical-specific information is available. Synthetic addition polymers of this type are generally high to very high molecular weight species. Water solubility is expected to be low based on the predominantly hydrophobic structure of the substance.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for poly(vinyl acetate)-poly(vinyl alcohol) polymer.

NICNAS has assessed poly(vinyl acetate)-poly(vinyl alcohol) polymer in an IMAP Tier 1 assessment and considers it a polymer of low concern, and concluded that it poses no unreasonable risk to human health and the environment[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Polymers with a molecular weight greater than 1,000 g/mol generally have a negligible vapor pressure, which indicates that the chemical is likely to exist solely as particulate matter in the atmosphere. As particulate matter, atmospheric oxidation is not expected to be a significant route of environmental removal. Likewise, volatilization from water or moist soil is not expected to occur at an appreciable rate (USEPA, 2013).

Non-ionic polymers such as poly(vinyl acetate)-poly(vinyl alcohol) polymer are not expected to be highly soluble in water based on its predominantly hydrophobic structure. If discharged to the aquatic environment, this polymer is expected to partition to soil or sediment. It is not expected to be highly mobile if released to the soil compartment (Beothling and Nabholz 1997).

Vinyl polymers not expected to undergo rapid degradation. In an OECD 302B (Zahn Wellens) test carried out using poly(vinyl acetate)-poly(vinyl alcohol) polymer, the test substance was found to be less than 10 % degraded after 28 days, indicating essentially no degradation (RE) (Environment Canada, 2005). However, some bacterial species like *Pseudomonads and Sphingomonads* are known to efficiently degrade the substance. Additionally, some fungal species like *Penicillium sp.* and *Geotrichum fermentans WF9101* have also been reported to degrade the substance efficiently. Microbial enzymes like oxidase, hydrolase, and dihydrogenase play an important role in the degradation of poly(vinyl acetate)-poly(vinyl alcohol) polymer (Amann and Minge, 2012).

The high molecular weight of the polymer is expected to preclude or minimize bioaccumulation. Polymers with a number average molecular weight (NAMW) greater than 1,000 g/mol cannot cross biological membranes (Boethling and Nabholz 1997).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=25213-24-5%2C+

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

No data on the environmental effects of the polymer were found. However, the high molecular weight of the substance is expected to negate or limit the bioavailability of the substance thus minimizing toxic effects on environmental receptors.

A. Aquatic Toxicity

No ecotoxicity data was identified for poly(vinyl acetate)-poly(vinyl alcohol) polymer. Information on Non-Ionic Polymers Group (DoEE, 2017) is provided below.

> *"Non-ionic polymers with low water solubility, such as the methyl acrylate-vinylidene chloride copolymer, generally have low toxicity to aquatic life (Beothling and Nabholz 1997). Insoluble non-ionic polymers have low bioavailability and their adverse effects result from physical. effects such as occlusion of respiratory organs (e.g. the gills of fish). These adverse effects occur only at very high loading levels in water (Beothling and Nabholz 1997).*
>
> *Water soluble or dispersible non-ionic polymers, such as polyacrylamide, are also typically of low concern for ecotoxicity. Non-ionic polymers with NAMW greater than 1 000 cannot be absorbed across biological membranes in aquatic organisms, and therefore toxicity only occurs through indirect effects such as chelation of essential nutrients (Beothling and Nabholz 1997). However, the structure of polyacrylamide suggests that it will have low potential to act by this mode of action. This is further supported by median effective concentration (EC50) and median lethal concentration (LC50) values available for other water soluble or dispersible non-ionic polymers, which are greater than 100 mg/L (Beothling and Nabholz 1997).*
>
> *Water soluble or dispersible polymers with NAMW less than 1 000 Da, or significant levels of LMW substances and trapped monomers, are of potential concern because of their increased bioavailability. However, this assessment was conducted assuming that the polymers in this group have NAMW greater than 1 000 Da and the percentage of LMW species is low."*

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Poly(vinyl acetate)-poly(vinyl alcohol) polymer is not expected to be biodegradable. Thus, it meets the criteria for persistence.

Poly(vinyl acetate)-poly(vinyl alcohol) polymer is not expected to bioaccumulate. Polymers with a NAMW greater than 1,000 g/mol cannot cross biological membranes (Boethling and Nabholz 1997). Thus, it does not meet the screening criteria for bioaccumulation.

There are no acute or chronic toxicity studies on poly(vinyl acetate)-poly(vinyl alcohol) polymer. However, the high molecular weight of the substance is expected to negate or limit the bioavailability of the substance thus minimizing toxic effects on environmental receptors.Thus, poly(vinyl acetate)-poly(vinyl alcohol) polymer does not meet the criteria for toxicity.

The overall conclusion is that poly(vinyl acetate)-poly(vinyl alcohol) polymer is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for poly(vinyl acetate)-poly(vinyl alcohol) polymer.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Poly(vinyl acetate)-poly(vinyl alcohol) polymer	25213-24-5	Not a PBT	No	Yes	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Amann, Manfred and Oliver Minge 2012. Biodegradability of Poly(vinyl acetate) and Related Polymers. Adv Polym Sci (2012) 245: 137–172

Boethling, RS, and Nabholz, JV 1997, 'Environmental assessment of polymers under the US Toxic Substances Control Act', in Hamilton J and Sutcliffe R (eds), Ecological assessment of polymers: strategies for product stewardship and regulatory programs, Van Nostrand Reinhold, New York, USA, pp 187-234.

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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Environment Canada. (2005). Canada's Domestic Substance List. https://canadachemicals.oecd.org/Search.aspx

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

United States Environmental Protection Agency (USEPA). (2013). Interpretive Assistance Document for Assessment of Polymers: Sustainable Futures Summary Assessment. June 2013.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency

EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

PORTLAND CEMENT

This dossier on Portland cement presents the most critical studies pertinent to use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Portland cement is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Portland cement is produced from limestone, shells and chalk or marl combined with shale, clay, slate, blast furnace slag, silica sand and iron ore. When heated at high temperatures, these ingredients form a rock-like substance that is then ground into a fine powder (with gypsum and limestone).

Portland cement is the most common type of cement in general use around the world as a basic ingredient of concrete, mortar, stucco and non-specialty grout. Portland cement clinker is a hydraulic material which, per ASTM standards, shall consist of at least two-thirds by mass of calcium silicates, (3 CaO·SiO2, and 2 CaO·SiO2), the remainder consisting of aluminium- and iron-containing clinker phases and other compounds. The ratio of CaO to SiO2 shall not be less than 2.0. The magnesium oxide content (MgO) shall not exceed 5.0% by mass.

When Portland cement is mixed with water, the anhydrous calcium silicates and other constituents in Portland cement react chemically with the water, creating a paste with water that binds with sand and rock to harden.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Portland Cement

CAS RN: 65997-15-1

Molecular formula: Not applicable.

Molecular weight: Unknown

Synonyms: Portland cement, cement kiln dust; kiln baghouse dust; kiln precipitator catch; Portland cement kiln; waste kiln dust

3 PHYSICO-CHEMICAL PROPERTIES

Portland cement is a fine, grey powder. Some main constituents of the substance (cement clinker phases) react with water and form water stable, highly insoluble hydration products. They are not volatile under ambient conditions. The melting points of calcium silicates exceed 700 ^{0}C. Density for related substance flue dust, Portland cement (CAS No. 68475-76-3) is 2,800 kg/m3 at 20 ^{0}C (ECHA).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for Portland cement.

NICNAS has assessed Portland cement in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Portland cement contains inorganic substances that are not applicable to biodegradation or bioaccumulation.

6 ENVIRONMENTAL EFFECTS SUMMARY

Toxicity studies are not available for Portland cement. Acute and chronic toxicity studies on similar substance flue dust, Portland cement suggest that these compounds have low aquatic toxicity. Likewise, they are virtually non-toxic to terrestrial organisms.

A. Aquatic Toxicity

Acute Studies

No data are available for Portland cement. Table 2 lists the results of acute aquatic toxicity studies on similar compound flue dust, Portland cement (CAS No. 68475-76-3).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=65997-15-1

Table 2 Acute Aquatic Toxicity Studies on Flue Dust, Portland Cement

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hour LC_{50}	11.1	1	ECHA
Daphnia magna	48-hour EC_{50}	>100*	1	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	28.2	1	ECHA

At the water accommodated fraction (WAF)*

Chronic Studies

No data are available for Portland cement. A study is available on flue dust, Portland cement (CAS No. 68475-76-3). The 21-day NOEC in a *Daphnia* reproduction test was 50 mg/L (ECHA) [Kl. Score = 1].

B. Terrestrial Toxicity

No data are available for Portland cement.

The 14-day NOEC of flue dust, Portland cement (CAS No. 68475-76-3) to earthworms is 1,000 mg/kg. Since 1,000 mg/kg is the limit dose, it is assumed that the LC50 is >1,000 mg/kg (ECHA) [Kl. Score = 1].

Terrestrial plant toxicity are available for flue dust, Portland cement (CAS No. 68475-76-3). The NOEC value for the emergence and early growth stages of oats (*Gramineae)*, rape (*Brassicaceae*) and soybean (*Leguminosae*) was 1,000 mg/kg (ECHA) [Kl. Score = 1].

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Portland cement is composed of naturally-occurring inorganic substances. The persistence criterion is not relevant to Portland cement.

Portland cement is not expected to bioaccumulate due to its low potential for bioavailability and low water solubility. Moreover, Portland cement will combine with sand and rock to form a paste and harden in the presence of water.

No aquatic toxicity studies are available for Portland cement. It is expected to be a low concern of toxicity to aquatic organisms because of its low potential for bioavailability and water insolubility. The NOEC from chronic aquatic toxicity studies on flue dust, Portland cement, a similar compound, is >0.1 mg/L. The acute $E(L)C_{50}$ values for flue dust, Portland cement are >1 mg/L in fish, invertebrates and algae. Thus, Portland cement is not expected to meet the criteria for toxicity.

The overall conclusion is Portland cement is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for Portland cement.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Portland Cement	64787-97-9	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

POTASSIUM BORATE

This dossier presents the most critical studies pertinent to the risk assessment of potassium borate as it relates to its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all the available data. Most of the information presented in this dossier was obtained from the ECHA database which provides information on chemicals that have been registered under the EU REACH (ECHA) framework. Where possible, the study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion- Potassium borate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Potassium borate is a salt of boric acid. Boric acid is produced when potassium borate is dissolved in water. In the environment, boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal conditions. Although some partitioning from water to soil and sediment can occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5-9.0, NICNAS 2019).

Potassium borate is reportedly used as a buffering agent in a variety of products used for landscaping, wood fire proofing, and various other domestic uses. Potassium borate exhibits low acute and chronic toxicity to aquatic organisms.

2 CHEMICAL AND IDENTIFICATION

Chemical Name (IUPAC): Dipotassium tetraborate

CAS RN: 1332-77-0

Molecular formula: $B_4K_2O_7$

Molecular weight: 313.4 g/mol

Synonyms: boric acid dipotassium salt, boron potassium oxide, potassium tetraborate, potassium borate, dipotassium tetraborate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for potassium borate are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Potassium Borate

Property	Value	Klimisch score	Reference
Physical state at 20^{o}C and 101.3 kPa	White odourless crystalline solid	1	ECHA
Melting Point	500 ^{o}C @ 101.3 kPa	1	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	-	-	-
Density	1911 kg/m^3 at 20 °C	1	ECHA
Vapour Pressure	Negligible at 20 °C	-	PubChem
Partition Coefficient (log K_{ow})	0.175	-	PubChem
Water Solubility	1-10 g/L @ 20 °C	1	ECHA
Dissociation constant (pKa)	9.08	1	ECHA

Boron is almost exclusively found in the environment in the form of boron-oxygen compounds, which are often referred to as borates. The high strength of the B-O bond relative to those between boron and other elements makes boron oxide compounds stable compared to nearly all non-oxide boron materials. Indeed, the B-O bond is among the strongest found in the chemistry of naturally occurring inorganic substances (ECHA).

In the environment, the chemicals in this group will dissociate and/or hydrolyse to release boron as boric acid [B(OH) (also formulated as H BO)] and/or borate anions (NICNAS, 2019).

Exposure to borates are often expressed in terms of boron (B) equivalents based on the fraction of boron in the source substance on a molecular weight basis. The B equivalents used are a generic designation rather than a designation of the element boron. The factor for converting potassium borate to B-equivalents is 0.185.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). Potassium borate is listed on the Australian Inventory of Chemical Substances-ACIS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for potassium borate.

NICNAS has assessed potassium borate in an IMAP Tier 1 assessment and it was concluded that this chemical poses no unreasonable risk to the environment provided that ANZECC water quality guidelines for physical and chemical stressors are not exceeded[1].

Table 2 Existing International Controls

Convention, Protocol, or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=1332-77-0

Convention, Protocol, or other international control	Listed Yes or No?
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE PROPERTIES

A. Summary

Potassium borate as a natural element is not degradable. It is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

B. Partitioning

Chemicals in this group will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions. Boric acid is highly water soluble and it tends to remain in surface waters. Although some partitioning from water to soil and sediment does occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5 to9.0) (NICNAS, 2019).

C. Biodegradation

Degradation is not applicable to inorganic borates, such as potassium borate. It is not subject to hydrolysis, photodegradation, or biodegradation (ECHA). Inorganic borates are subject to chemical transformation processes (adsorption, complexation, precipitation, fixation) once released into the environment (ECHA).

D. Environmental Distribution

The Kp value for potassium borate was calculated as the median of all measured Kp values from the GEMAS project (Geochemical Mapping of Agricultural and Grazing Land Soil project): 2.19 L/kg dry weight (ECHA) [KI. Score = 2]. The chemistry of boron in soils and aquatic systems is simplified by the absence of oxidation- reduction reactions or volatilization. Redox processes can mobilize Fe oxides and Mn oxides, which may lead to a release of boron in aquatic systems. Generally, sediments are characterised with higher pH values than the soil matrix, which increases the boron sorption capacity (ECHA).

If released to soil, based on this low Kp value, low vapour pressure and high water solubility, potassium borate is considered relatively mobile in the environment, under certain conditions (ECHA).

E. Bioaccumulation

The WHO review of boron (WHO, 1998) noted that "highly water soluble materials are unlikely to bioaccumulate to any significant degree and that borate species are all present essentially as un-dissociated and highly soluble boric acid at neutral pH". A BCF of <0.1-10.5 L/kg has been reported for potassium borate in fish and oysters (ECHA) [Kl. Score = 2]. This data suggests that potassium borate does not bioaccumulate in the aquatic environment.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Potassium borate is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

In ecotoxicological tests for boron, the exposure concentrations are expressed as boron equivalents i.e. mg B/L. This is because boric acid and borate salts will have the same boron speciation when dissolved in environmental matrices. Therefore, in the following sections toxicological values are given as mg B/L regardless of the form of boron that was tested.

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on potassium borate.

Table 3 Acute Aquatic Toxicity Studies on Potassium Borate

Test Species	Endpoint	Results (mg/L)*	Klimisch score	Reference
Pimephales promelas (Fathead minnow)	96-hr LC_{50} (mortality)	79.7	1	ECHA
Daphnia magna (Daphnid)	48-hr LC_{50} (mortality)	133	1	ECHA
Pseudokirchneriella subcapitata (Algae)	72-hr EC_{50} (biomass)	40	1	ECHA

*Values reported in mg B/L.

Chronic Studies

Table 4 lists the results of key chronic aquatic toxicity studies conducted on potassium borate.

Table 4 Chronic Aquatic Toxicity Studies on Potassium Borate

Test Species	Endpoint	Results (mg/L)*	Klimisch score	Reference
Brachydanio rerio	34-d NOEC (mortality)	5.6	1	ECHA
Pimephales promelas (Fathead minnow)	32-d NOEC (mortality)	11.2	1	ECHA
Brachionus calyciflorus (Rotifera)	72-hr NOEC (mortality)	24.6	1	ECHA
Daphnia magna	21-day NOEC (reproduction)	10	1	ECHA
Pseudokirchneriella subcapitata (Algae)	72-hr NOEC (growth rate)	17.5	1	ECHA

*Values reported in mg B/L.

The ANZG water quality guideline (2021) derived a very high reliability default guideline value (DGVs) for (dissolved) boron in freshwater from 22 chronic (long-term) toxicity data, comprising eight fish, two amphibians, three crustaceans, one bivalve, three macrophytes, one green microalga, three diatoms and one blue–green alga. The summary of representative data used by ANZG to develop a water quality guideline for boron is presented in Table 5 below. These values are noted to be consistent with those reported in ECHA. Additional chronic aquatic toxicity data is found in the ANZG Technical Brief (ANZG, 2021).

Table 5 Chronic Aquatic Toxicity Studies on Boron[1]

Test Species	Endpoint	Results (mg/L)
Danio rerio	34-day NOEC (Biomass)	1.8
Pimephales promelas	32-day NOEC (Mortality)	11
Daphnia magna	14-day NOEC (Reproduction)	2.4
Pseudokirchneriella subcapitata	4-day NOEC (Growth)	2.8

1 - The DGVs are based on toxicity data for boron as either boric acid, H_3BO_3 (CAS 10043-35-3), or borax, $Na_2B_4O_710H_2O$ (CAS 1303-96-4), in freshwater.

In the chronic toxicity data set, fish sensitivity to boron ranged from the least sensitive species in the dataset (*Melanotaenia splendida*, LC10 102 mg/L) to the third most sensitive species in the dataset (*Danio rerio*, NOEC 1.8 mg/L). Of the crustaceans, *D. magna* was best represented in the literature, with

18 published NOEC values (ranging from 2.4 mg/L to 29 mg/L) for six different endpoints from six different publications. The final NOEC of 2.4 mg/L used in the DGV derivation was lower than that for *C. dubia* (NOEC 5.6 mg/L) and for the amphipod *H. azteca* (NOEC 6.6 mg/L).For *P. subcapitata*, there were three separate studies available with toxicity data for boron. The toxicity values from these studies ranged from a NOEC of 2.8 mg/L to a NEC of 27 mg/L, varying with endpoint, duration and test medium used. Boron was least toxic to *P. subcapitata* when tested in algal growth medium with added $NaHCO_3$, suggesting that carbonate addition may have influenced boron toxicity. Therefore, although NECs are preferred to NOECs or EC10s (Warne et al. 2018), in this instance, a reliable NOEC of 2.8 mg/L was the most sensitive toxicity value for *P. subcapitata* (ANZG, 2021).

C. Terrestrial Toxicity

Ecotoxicological tests with plants and soil invertebrates have recorded modest chronic toxicity values (NOECs/ECs) in the range of 15.3 to 84.0 and 5.2 to 315 mg total B/kg, respectively (ECHA, 2008). However, to predict the potential toxicity of boron to plants and soil organisms, measuring the total boron concentration may be unsuitable. Instead, potential toxicity is better predicted using boron concentrations in the soil solution (extractable boron) (Mertens, et al., 2011). In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron (NICNAS, 2019).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium borate dissociates into an inorganic compound known as boric acid. Biodegradation is not applicable to this inorganic compound since it ubiquitous in the soil and sediment. For this PBT assessment, the persistent criteria are not considered applicable in regard to potassium borate.

A BCF of <0.1-10.5 L/kg has been reported for potassium borate in fish and oysters. This data suggests that potassium borate does not bioaccumulate in the aquatic environment. Thus, it does not meet the criteria for bioaccumulation.

The chronic toxicity data on potassium borate has a NOEC > 0.1 mg/L. The acute LC50 values are greater than 1 mg/L. Thus, this substance does not meet the criteria for toxicity.

The overall conclusion is that potassium borate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium borate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Potassium Borate	1332-77-0	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 1 - Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS, AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union

g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NEC	no effect concentration
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

POTASSIUM CHLORIDE

This dossier on potassium chloride presents the most critical studies pertinent to the risk assessment of potassium chloride in its use in drilling muds and hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on potassium chloride (OECD, 2001a,b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Potassium chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Potassium chloride (KCl) dissociates completely in aqueous solutions to potassium (K+) and chloride (Cl-) ions. Potassium chloride and its dissociated ions are ubiquitous in the environment. Potassium (K+) and chloride (Cl-) ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Neither potassium chloride nor its dissociated ions are expected to bioaccumulate. Potassium chloride is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Potassium chloride

CAS RN: 7447-40-7

Molecular formula: KCl

Molecular weight: 74.55 g/mol

Synonyms: Potassium chloride

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Potassium Chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid; white crystals	2	ECHA
Melting Point	770°C @ 101.3 kPa	1	ECHA
Boiling Point	1,407°C (pressure not provided)	2	OECD, 2001a,b
Density	1984 kg/m^3	2	ECHA
Partition Coefficient (log K_{ow})	-	-	-

Property	Value	Klimisch score	Reference
Water Solubility	255 g/L @ 25°C	2	Lide, 2009; ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for potassium chloride.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Potassium chloride (KCl) dissociates completely in aqueous solutions to potassium (K^+) and chloride (Cl^-) ions. Potassium chloride and its dissociated ions are ubiquitous in the environment.

The transport and/or leaching of potassium (K^+) and chloride (Cl^-) ions is affected by clay minerals (type and content), pH, and organic matter. Potassium ions are less mobile and less prone to leaching than anions in soil, such as chloride and nitrate (NO_3^-). Chloride binds only weakly to soil particles, and therefore follows water movement (OECD, 2001b).

Potassium (K^+) and chloride (Cl^-) ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated (OECD, 2001b; Ganong, 1995). Neither potassium chloride nor its dissociated ions are expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Potassium chloride is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

The results of the acute toxicity studies conducted on potassium chloride are presented in Table 3.

Table 3 Acute Aquatic Toxicity Studies on Potassium Chloride

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	880	2	Mount et al., 1997; ECHA
Daphnia magna	48-hour EC_{50}	660	2	Mount et al., 1997; ECHA
Ceriodaphnia dubia	48-hour EC_{50}	630	2	Mount et al., 1997; ECHA
Scenedesmus subspicatus	72-hour EC_{50}	>100* (growth rate)	1	ECHA

*NOEC ≥ 100 mg/L

Chronic Studies

In a fish early-life-stage test with the fathead minnow (*Pimephales promelas*), the 7-day NOEC was 500 mg/L (ECHA).

C. Terrestrial Toxicity

No studies were identified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium chloride is an inorganic salt that dissociates completely to potassium and chloride ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both potassium and chloride ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Potassium and chloride ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Therefore, potassium chloride is not expected to bioaccumulate.

There are no adequate chronic aquatic toxicity studies available on potassium chloride. The acute EC_{50} values for potassium chloride are >1 mg/L in fish, invertebrates and algae. Therefore, potassium chloride does not meet the screening criteria for toxicity.

The overall conclusion is that potassium chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium chloride.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Potassium Chloride	7747-40-7	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union

g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

POTASSIUM HYDROXIDE

This dossier on potassium hydroxide presents the most critical studies pertinent to the risk assessment of potassium hydroxide in its use in drilling muds and water treatment systems. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the OECD-SIDS documents on potassium hydroxide (OECD, 2002) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Potassium hydroxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Potassium hydroxide (KOH) is a strong alkaline substance that dissociates completely in water to potassium (K+) and hydroxyl (OH-) ions. Both ions are ubiquitous in the environment. K+ and OH- ions will not adsorb on the particulate matter or surfaces and will not accumulate in living tissues. Potassium is an essential nutrient involved in fluid and electrolyte balance and is required for normal cellular function. The hazard of KOH for aquatic organisms is caused by the hydroxyl ion (OH-) which has the potential to increase the pH of the aquatic environment, depending on the buffering capacity of the water.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Potassium hydroxide

CAS RN: 1310-58-3

Molecular formula: KOH

Molecular weight: 56.1 g/mol

Synonyms: Potassium hydroxide; caustic potash; potash lye; potassium hydrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Potassium Hydroxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	2	ECHA
Melting Point	406°C (pressure not provided) 250°C	2	ECHA
Boiling Point	1,327°C @ 1013 hPa	2	ECHA

Property	Value	Klimisch score	Reference
Density	2044 kg/m^3 @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	Very soluble	2	ECHA

Potassium hydroxide (KOH) is a strong alkaline substance that dissociates completely in water to potassium (K^+) and hydroxyl (OH^-) ions.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for potassium hydroxide.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Due to its high water solubility and low vapour pressure, potassium hydroxide will be found predominantly in the aquatic environment where it dissociates completely to potassium (K^+) and hydroxyl (OH^-) ions. Both ions are ubiquitous in the environment (UNEP, 1995).

The addition of potassium hydroxide to an aquatic ecosystem may increase the pH depending on the buffer capacity of the receiving water. In general, the buffer capacity is regulated by the equilibria between CO_2, HCO_3^- and CO_3^{2-}:

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ ($pKa_1 = 6.35$)
$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ ($pKa_2 = 10.33$)

A release of potassium hydroxide into the aquatic environment from the use of KOH could potentially increase the potassium concentration and the pH in the aquatic environment. Table 3 shows the concentration of potassium hydroxide needed to increase the pH to values of 9.0, 10.0, 11.0 and 12.0.

Table 3 Potassium Hydroxide Concentration (mg/L) Needed to Increase pH to a Value of 9 (OECD, 2002)

Buffer capacity	Concentration of KOH (mg/L)
0 mg/L HCO_3 (distilled water)	0.56
20 mg/L HCO_3 (10^{th} percentile of 77 rivers)	0.86
106 mg/L HCO_3^- (mean value of 77 rivers)	4.51
195 mg/L HCO_3^- (90^{th} percentile of 77 rivers)	8.30

K^+ and OH^- ions will not adsorb on the particulate matter or surfaces and will not accumulate in living tissues (OECD, 2002).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Aquatic Toxicity

As noted in(OECD, 2002) toxicity tests with KOH depend on the buffer capacity of the test medium. Thus, the pH change could influence the speciation of other chemicals and therefore increase and/or decrease the toxicity.

There are no guideline studies on potassium hydroxide; the studies summarised below have Klimisch scores of 3 or 4. Studies on sodium hydroxide (NaOH) have also been included, given its similarity to KOH.

Acute Fish

KOH: The 96-hour LC_{50} to *Gambusia affinis* (mosquito fish) is 80 mg/L. At 56 mg/L, no mortality was observed.

NaOH: The 24-hour LC_{50} to *Carassius auratus* (goldfish) is 160 mg/L. At 100 mg/L, which was equivalent to a pH of 9.8, no mortality was observed. The 48-hour LC_{50} to *Leuciscus idus melanotus*, is 189 mg/L. The 96-hour LC_{50} of *Gambusia affinis* (mosquitofish) is 125 mg/L. At 84 mg/L, no effects on the fish were observed. The pH was 9 at 100 mg/L.

Acute Invertebrate

KOH: No studies are available.

NaOH: The 48-hour LC_{50} is 40 mg/L for *Ceriodaphnia cf. dubia*. The toxicity threshold concentration of NaOH for *Daphnia magna* was reported to range from 40 to 240 mg/L.

Acute Algae

No studies are available.

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium hydroxide is an inorganic salt that dissociates completely to potassium and hydroxide ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both potassium and hydroxide ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Potassium and hydroxide ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Thus, potassium hydroxide is not expected to bioaccumulate.

No chronic toxicity data exist on potassium hydroxide; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Thus, potassium hydroxide does not meet the screening criteria for toxicity.

The overall conclusion is that potassium hydroxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium hydroxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Potassium Hydroxide	1310-58-3	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regulatory Toxicology and Pharmacology 25:1-5.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
Pa	pascal

PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

POTASSIUM PYROPHOSPHATE

This dossier on potassium pyrophosphate presents the most critical studies pertinent to the risk assessment of potassium pyrophosphate in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Potassium pyrophosphate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Potassium pyrophosphate dissociates completely in aqueous media to potassium ions (K+) and pyrophosphate ions ($P_2O_7^{4-}$). The pyrophosphate anion is unstable in aqueous solution and hydrolyses into inorganic phosphate. Both potassium ions (K+) and phosphate ions (HPO_4^{2-}) are ubiquitous in the environment. Both ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Neither potassium pyrophosphate nor its dissociated ions are expected to bioaccumulate. Potassium pyrophosphate is expected to be of low toxicity concern to aquatic organisms based on a similar compound.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): tetrapotassium (phosphonooxy)phosphonate

CAS RN: 7320-34-5

Molecular formula: $K_4O_7P_2.4K$

Molecular weight: 330.33 g/mol

Synonyms: Tetrapotassium diphosphate;potassium pyrophosphate; potassium diphosphate; tetrapotassium diphosphate; TKPP; tetrapotassium pyrophosphate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Potassium Pyrophosphate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, granular solid	1	ECHA
Melting Point	>569°C (pressure not provided)	4	ECHA
Boiling Point	-	-	-
Density	2610 kg/m^3 @ 20°C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	-	-	-
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	10 g/L@ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for potassium pyrophosphate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Potassium pyrophosphate dissociates completely in aqueous media to potassium ions (K^+) and pyrophosphate ions ($P_2O_7^{4-}$). The pyrophosphate anion is unstable in aqueous solution and hydrolyses into inorganic phosphate:

$P_2O_7^{4-} + H_2O \rightarrow 2HPO_4^{2-}$.

Both potassium ions (K^+) and phosphate ions (HPO_4^{2-}) are ubiquitous in the environment. Both ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated (Ganong, 1995). Neither potassium pyrophosphate nor its dissociated ions are expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Potassium pyrophosphate is expected to be of low toxicity concern to aquatic organisms based on a similar compound.

B. Aquatic Toxicity

Acute Studies

There are no acute fish or algal toxicity studies on potassium pyrophosphate. Data from phosphoric acid, potassium salt (2:3), dehydrate (CAS No. 6922-99-4) will be used as read-across to potassium pyrophosphate.

The 96-hour LC_{50} of phosphoric acid, potassium salt (2:3), dehydrate (CAS No. 6922-99-4) to rainbow trout (*Oncorhynchus mykiss*) is >100 mg/L based on growth rate (ECHA). [Kl. score = 2]

The 48-hour EC_{50} of potassium pyrophosphate to *Daphnia magna* is >100 mg/L (ECHA). [Kl. score = 1]

The 72-hour EC_{50} of phosphoric acid, potassium salt (2:3), dehydrate (CAS No. 6922-99-4) to *Selenastrum capricornutum* is >100 mg/L based on growth rate (ECHA). [Kl. score = 2]

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium pyrophosphate is an inorganic salt that dissociates completely to potassium and pyrophosphate ions (and ultimately to phosphate ions) in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both potassium and phosphate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Potassium and phosphate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Therefore, potassium pyrophosphate is not expected to bioaccumulate.

There are no chronic aquatic toxicity data available on potassium pyrophosphate. The acute EC_{50} values for potassium pyrophosphate are >1 mg/L in fish, invertebrates and algae. Therefore, potassium pyrophosphate does not meet the screening criteria for toxicity.

The overall conclusion is that potassium pyrophosphate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium pyrophosphate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Potassium Pyrophosphate	7320-34-5	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Ganong, W.F. (1995). Review of Medical Physiology, 17th Edition, Appleton & Lange, Norwalk, Connecticut, USA.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
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EC	effective concentration
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g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
Kl	Klimisch scoring system
kg/m^3	Kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

POTASSIUM SULPHATE

This dossier on potassium sulphate presents the most critical studies pertinent to the risk assessment of the substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Potassium sulphate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Potassium sulphate is an inorganic compound predominantly used as a fertilizer. In aqueous solution, potassium sulphate is completely dissociated into the potassium ion (K+) and the sulfate anion (SO_4^{2-}). Biodegradation is not applicable to inorganic compounds and potassium sulphate is not expected to adsorb or bioaccumulate to a significant extent. Potassium sulphate is of low toxicity concern to aquatic receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): dipotassium sulphate

CAS RN: 7778-80-5

Molecular formula: K_2SO_4

Molecular weight: 174.26 g/mol

Synonyms: Potassium bisulphate, Potassium bisulphate, Potassium hydrogen sulphate, Potassium hydrogensulphate, Potassium hydrosulphate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Potassium Sulphate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	colorless or white, odorless, hard, bitter crystals, or white granules or powder	2	ECHA
Melting Point	1067 °C at 101.3 kPa	2	ECHA
Boiling Point	1689 °C (pressure not provided)	4	ECHA
Density	2660 kg/m^3 @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Water Solubility	120 g/L @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for potassium sulphate.

NICNAS has assessed potassium sulphate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health and the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

In aqueous solution, potassium sulphate is completely dissociated into the potassium ion (K+) and the sulfate anion (SO_4^{2-}). Biodegradation is not applicable to inorganic compounds. Based on the high water solubility and the ionic nature, potassium sulphate is not expected to adsorb or bioaccumulate to a significant extent. High mobility in soil is also to be expected. However, due to ion-ion interactions it is to be expected that mobility in soil is significantly reduced. Potassium sulphate will not volatilize from soil (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Potassium sulphate is of low toxicity concern to aquatic receptors.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=64-18-6%2C+

A. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on potassium sulphate.

Table 3: Acute Aquatic Toxicity Studies on Salts of Potassium sulphate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fathead minnow	96-hr LC_{50}	680	2	ECHA
Daphnia magna	48-hr EC_{50}	720	2	ECHA
Chlorella vulgaris	72-hr EC_{50}	2700	2	ECHA

Chronic Studies

No studies are available.

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium sulphate dissociates completely to potassium and sulphate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistence criteria is not considered applicable.

Based on the high water solubility and the ionic nature, potassium sulphate is not expected to adsorb or bioaccumulate to a significant extent. Thus, potassium sulphate does not meet the criteria for bioaccumulation.

There are no chronic toxicity studies on potassium sulphate. The acute toxicity values for three species are > 1 mg/L. Thus, potassium sulphate does not meet the criteria for toxicity.

The overall conclusion is that potassium sulphate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium sulphate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Potassium sulphate	7778-80-5	Not a PBT	No	No	NA	No	No	No	1	No data available	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

SILICIC ACID, POTASSIUM SALT

This dossier on silicic acid, potassium salt (potassium silicate) presents the most critical studies pertinent to the risk assessment of potassium silicate in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the OECD-SIDS documents on Soluble Silicates which includes potassium silicate (OECD, 2004), and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Silicic acid, potassium salt is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Silicic acid, potassium salt or potassium silicate is an amorphous glass, and it is solidified as a glass from the melt (solid or lump glasses). It is essentially anhydrous and differs from ordinary glasses in that it is soluble in water at elevated temperature and pressure leading to silicate solutions (liquid glasses). Both solid and liquid glasses are often referred to as waterglass. Silicate solutions are defined by their density and viscosity, which together with the MR defines a unique composition for the silicate solution. By evaporation of silicate solutions, fine powders or granules are obtained that have a residual water content of approximately 20%. Unlike ground lump glass, these materials dissolve readily in water to give silicate solutions (OECD, 2004).

Upon dissolution in water, potassium silicate forms potassium ions (K+) and molecular speciation of silicates. Depending on both pH and concentration the respective solutions contain varying proportions of monomeric tetrahydral ions, oligomeric linear or cyclic silicate ions (OECD, 2004).

Silicic acid, potassium salt or potassium silicate is an amorphous glass in the form of fine powders or granules. As an inorganic substance, it is not amenable to biodegradation; it is not expected to bioaccumulate. Potassium silicate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Potassium hydroxyl(oxo)silanolate

CAS RN: 1312-76-1

Molecular formula: K2O · nO2Si

Molecular weight: 248.44 g/mol (tetrapotassium orthosilicate); soluble silicates are not generally stoichiometric chemical substances (with a specific chemical formula and molecular weight), but rather glasses or aqueous solutions of glasses.

Synonyms: Potassium silicate; potassium waterglass; potassium polysilicate; silicic acid, potassium salt; soluble potash glass

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Potassium Silicate

Property	Value	Klimisch score	Reference
Physical state	Amorphous glass melt; aqueous solution of spray-dried powder with ~20% residual water	-	OECD, 2004
Flow Point	905°C	2	ECHA
Density	1260 – 1600 kg/m^3 (solution) @ 20°C; 750 kg/m^3 spray-dried powder	2	ECHA
Vapour Pressure	Negligible at ambient temperature	-	OECD, 2004
Partition Coefficient (log K_{ow})	Not relevant	-	OECD, 2004
Water Solubility	Solution: infinitely miscible; spray-dried solution: readily dissolvable	-	OECD, 2004

*Due to their glass nature, solid amorphous silicates do not have discrete melting points but rather flow points.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for silicic acid, potassium salt.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Potassium silicate readily dissolves in water to potassium ions (K^+) and molecular speciation of silicates. Dissolved silica from commercial soluble silicates is indistinguishable from natural dissolved silica. Silica (SiO_2) represents about 59% of the elemental composition of the earth's crust. Similar percentages are obtained for many sediments and soils (Jackson, 1964). Compounds of silicon and oxygen are ubiquitous in the environment; they are present in inorganic matter (i.e., minerals and soils) and in organic matter.

Silica is found in all natural waters and the median values in the United States were reported to be 17 mg SiO_2/L for ground waters and 14 mg SiO_2/L for streams (Davis, 1964). The world-wide concentration in rivers is 13 mg SiO_2/L (Edwards and Liss, 1973).

Potassium silicate is an inorganic substance and therefore not amenable to biodegradation. It is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Potassium silicate is of low toxicity concern to aquatic organisms. All of the available aquatic ecotoxicity tests with potassium silicate and with sodium silicate (used as read-across for algae) show toxicity at concentrations well above 100 mg/L.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on potassium silicate.

Table 3 Acute Aquatic Toxicity Studies on Potassium Silicate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Leuciscus idus	48-hour LC_{50}	>146	2	OECD, 2004; ECHA
Daphnia magna	24-hour EC_{50}	>146	2	OECD, 2004; ECHA
Scenedesmus subspicatus	72-hour EC_{50}	207* (biomass)	2	OECD, 2004; ECHA

*Test material was sodium silicate (CAS No. 1344-09-8).

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

A honey bee acute contact toxicity study performed per (USEPA OCSPP 850.3020) was conducted on AgSil™ 25 potassium silicate solution (29.1% potassium silicate in water). The 48-hour LD_0 was 25 µg/animal and the 48-hour LD_{50} was 25 µg/animal (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Potassium silicate is an inorganic compound that dissociates completely to potassium and silicate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both potassium and silicate ions are also ubiquitous and are present in most water, soil and sediment. For the

purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic compound.

Potassium and silicate ions are essential to all living organisms and are ubiquitous in the environment. Therefore, potassium silicate is not expected to bioaccumulate.

No chronic toxicity data exist on potassium silicate; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Therefore, potassium silicate does not meet the screening criteria for toxicity.

The overall conclusion is that potassium silicate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for potassium silicate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Silicic Acid, Potassium Salt	1312-76-1	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Davis, S.N. (1964). Silica in streams and ground water. Am. J. Sci. 262: 870-891.

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

Edwards, A.M.C. and Liss, P.S. (1973). Evidence of buffering of dissolved silicon in fresh waters. Nature 243: 341-342.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

OECD. (2004). OECD SIDS Initial Assessment Report (SIAR) and IUCLID Data Set for Soluble Silicates, UNEP Publications. Available at: https://hpvchemicals.oecd.org/ui/handler.axd?id=3cb4f34b-2afa-4004-b447-521188909235

USEPA. (2012). Ecological Effects Test Guidelines. OCSPP 850.3020: Honey Bee Acute Contact Toxicity Test. January.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
LC	lethal concentration

LD	lethal dose
mg	milligram
OCSPP	Office of Chemical Safety and Pollution Prevention
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
USEPA	United States Environmental Protection Agency
µg	microgram

SILICON DIOXIDE

This dossier on silicon dioxide does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies pertinent to the risk assessment of silicon dioxide in its use in coal seam gas extraction activities. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on synthetic amorphous silica and silicates (OECD 2004), and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Silicon dioxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Synthetic amorphous silica (silicon dioxide) is produced by a wet process by reacting an aqueous alkali metal silicate solution and a mineral acid. An extensive hydrated silica structure, or "gel" is formed which is then dried (CAS No. 112926-00-8). A precipitated silica is also produced in a "wet" process in a finely-divided, hydrated form by precipitation from aqueous alkali metal silicate solutions (CAS No. 11296-00-8). This product contains no detectable crystalline silica.

Synthetic amorphous silica and silicates released into the environment are expected to be distributed mainly into soils and sediments, weakly into water and probably not at all in the air due to their physico-chemical properties, particularly low water solubility and very low vapour pressure (OECD, 2004). Biodegradation is not applicable to this inorganic substance and bioaccumulation is not expected. The substance is of low toxicity concern to aquatic or terrestrial receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): dioxosilane

CAS RN: 112926-00-8 (also CAS No. 7631-86-9 and CAS No. 112945-52-5)[1]

Molecular formula: SiO_2

Molecular weight: 60.08 g/mol

Synonyms: silicon dioxide; hydrated silica; synthetic amorphous silica; silica gel, crystal-free

[1] : Silicon dioxide (CAS No. 7631-86-9) is the general CAS No. which includes all forms of silicas (e.g. also crystalline and natural forms)

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Silicon Dioxide (CAS No. 7631-86-9)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White powder	1	ECHA
Melting Point	>529.6 °C @ 101.3 kPa	1	ECHA
Boiling Point	Not applicable	-	ECHA
Density	1,810 kg/m3 @ 20 °C (skeleton density)	1	ECHA
Water Solubility	0.1 – 0.13 g/L* (slightly soluble)	1	ECHA
Dissociation Constant (pKa)	6.65 @ 20 °C	2	ECHA

*Based on dissolved SiO_2.; surface-treated SAS does not differ from non-treated SAS

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for silicon dioxide.

Based on an assessment of environmental hazards, NICNAS identified the substance as a chemical of low concern to the environment (DoEE, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Amorphous silica is a naturally occurring substance. The synthetic form (synthetic amorphous silica, SAS) is of higher amorphous purity than the naturally occurring amorphous silica and does not contain contaminants. Both natural amorphous silica and SAS have the tendency to aggregate and agglomerate but are not expected to undergo any transformation in the atmospheric or terrestrial compartment, apart from dissolution by water and precipitation in sediments (ECHA).

Synthetic amorphous silica and silicates released into the environment are expected to be distributed mainly into soils and sediments, weakly into water and probably not at all in the air due to their physico-chemical properties, particularly low water solubility and very low vapour pressure (OECD, 2004).

Biodegradation is not applicable to this inorganic substance and bioaccumulation is not expected.

B. Partitioning

Based on the physico-chemical nature and structure of SAS, no photo- or chemical degradation is expected. The hydrolysis process is considered a rate-limiting step in the dissolution of SAS in water. Once released and dissolved into the environment no distinction can be made between the initial forms of silica (ECHA).

C. Biodegradation

Biodegradation is not applicable due to the chemical nature (inorganic substance) of silicon dioxide (ECHA).

D. Environmental Distribution

Due to its physico-chemical properties, SAS is expected to mainly distribute into soil and sediment, where it undergoes natural transformation processes of weathering including dissolution and precipitation. Amorphous silica dissolution has an essential role in controlling biogeochemical cycling of silicon (ECHA).

E. Bioaccumulation

At normal environmental pH, dissolved silica [$Si(OH)_4$] exists as orthosilicic acid which is the bioavailable form for aquatic organisms and plays an important role in the biogeochemical silicon cycle in the natural environment. Dissolved silica is a major nutrient for many aquatic systems and certain terrestrial plants. Due to its inherent physico-chemical properties, such as the absence of lipophilicity as well as the capability of organisms to eliminate absorbed SAS components, bioaccumulation is not expected (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance is of low toxicity concern to aquatic or terrestrial receptors.

A. Aquatic Toxicity

Acute Studies

Table 3: Acute Aquatic Toxicity Studies on Silicon Dioxide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-h LL_0	10,000*	1	ECHA
Danio rerio	96-h LL_0	10,000	1	ECHA
Daphnia magna	48-h EL_{50}	>1,000**	2	ECHA
Daphnia magna	24-h EL_{50}	>10,000	2	ECHA
Desmodesmus subspicatus	72-h EC_{50} 72-h NOEC	>173.1	1	ECHA

*Silica, amorphous, fumed, crystalline-free

**Mortality may have occurred may have occurred from physical effects of unfiltered medium.

Chronic Studies

There are no chronic studies for fish. Due to the known inherent physico-chemical properties, the absence of acute toxic effects as well as the ubiquitous presence of silica/silicates in the environment, there is no indication for harmful long-term effects arising from exposure to SAS (ECHA).

The 21 day-NOECs for daphnid reproduction were at 100 mg/L or higher for the dissolved fractions of SAS (ECHA) [Kl. Score = 1].

B. Terrestrial Toxicity

In GLP and guideline studies using earthworms, SAS showed no toxicity at exposures exceeding current maximum recommended test concentrations. The lowest NOECs for mortality and reproduction were at 50 g/kg soil (dw) and 25 g/kg soil (dw), respectively. At the effect levels (LC50s: 70 g/kg soil (dw) and higher; LOECs, reproduction: 50 g/kg soil(dw) and higher) the substrates were very dry and the effects secondary to exsiccosis (verified by histological examinations) (ECHA) [Kl. Score = 1].

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Biodegradation is not applicable to silicon dioxide, an inorganic substance. For the purposes of this PBT assessment, the persistent criteria is not considered applicable to silicon dioxide.

Due to its inherent physico-chemical properties, such as the absence of lipophilicity as well as the capability of organisms to eliminate absorbed SAS components, bioaccumulation is not expected. Thus, silicon dioxide does not meet the criteria for bioaccumulation.

The lowest chronic toxicity value for silicon dioxide is >0.1 mg/L. The acute E(L)C_{50} values for silicon dioxide across several species is >1 mg/L. Thus, it does not meet the criteria for toxicity.

The overall conclusion is that silicon dioxide (CAS No. 112926-00-8) is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for silicon dioxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Silicon Dioxide	112926-00-8	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy (DoEE). (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/kg	grams per kilogram
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration

mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

SODIUM ACETATE

This dossier on sodium acetate presents the most critical studies pertinent to the risk assessment of sodium acetate in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium acetate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium acetate is the salt of acetic acid, and acetic acid is widely used in the coal seam gas industry as a pH adjuster and for iron control (DoEE, 2017a).

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. Both of these chemical species are naturally occurring and ubiquitous in the aquatic environment. The acetate ion is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment. The acetate ion is of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium acetate

CAS RN: 127-09-3

Molecular formula: $C_2H_4O_2.Na$

Molecular weight: 82.03 g/mol

Synonyms: Acetic acid, sodium salt, Sodium acetate anhydrous, Acetic acid sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Acetate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	crystalline or white granular powder	1	ECHA
Melting Point	324 °C @ 101.3 kPa	1	ECHA
Boiling Point	Not applicable as substance is solid.	-	ECHA
Density	1530 kg/m^3 @ 20 °C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour pressure	Not applicable	-	ECHA
Partition Coefficient (log P_{ow})	-3.72	2	ECHA
Water Solubility	1,250 g/L @ 25 °C	1	ECHA
Dissociation Constant (pKa)	4.756	4	ECHA

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. Acetate is ubiquitous in natural water and acts as a key nutrient, supplying energy to heterotrophic algae under aerobic conditions. Acetate is also formed by anaerobic bacteria through natural fermentation processes as a source of energy. Sodium ions are similarly naturally ubiquitous in the environment (DoEE, 2017a).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium acetate.

Based on an assessment of hazards, NICNAS identified the substance as a chemical of low concern to human health and the environment (NICNAS, 2017 and DoEE, 2017b). Chemicals of low concern are considered to have a low likelihood of causing adverse human health effects should an exposure occur and are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. Both of these chemical species are naturally occurring and ubiquitous in the aquatic environment. The acetate ion is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment.

B. Partitioning

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. The pKa of sodium acetate (as acetic acid) is 4.76, indicating that this substance will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts (PubChem).

C. Biodegradation

The substance is considered readily degradable. The biodegradability was determined with a non adapted activated sludge for the test item over a test period of 28 days in the DOC-Die-Away test. At 7 days, the biodegradation reached the 86% and at 28 days the biodegradation reached the 99% (ECHA)[KI Score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017b).

D. Environmental Distribution

No experimental data are available for sodium acetate. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values from log K_{ow} is 1.0 L/kg (ECHA) [KI. Score = 2]. Based on this value, sodium acetate has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

Release of large volumes of sodium acetate (or acetic acid) to natural waterways may disturb the health of aquatic ecosystems through direct and indirect physical and chemical effects. For example, at very high concentrations, these chemicals have the potential to modify the pH beyond normal ranges. Further, rapid biodegradation of large quantities of these chemicals in natural water bodies may decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life. However, numerous natural biogeochemical mechanisms exist which tend to limit fluctuations in nutrient levels, which occur frequently in healthy aquatic ecosystems. (DoEE, 2017a).

E. Bioaccumulation

There are no reliable bioaccumulation studies on sodium acetate. The low Log K_{ow} (-3.72) suggests sodum acetate will not bioaccumulate to a substantial degree ((ECHA)[KI Score = 2].

Further, bioaccumulation of sodium acetate is not expected to occur because the substance dissociates completely in aqueous solution to acetate and its sodium ion. Both ions are ubiquitous in the environment. Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The acetate ion is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute

The aquatic toxicity data for sodium acetate are presented in Table 3.

Table 3. Acute Aquatic Toxicity Studies on Sodium Acetate

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Brachydanio rerio	96h-LC50	> 100 mg/L	2	ECHA
Daphnia magna	EC50 (48h)	>385.60	2	ECHA
Acartia tonsa	LC50 (48h)	2075.20	2	ECHA
Algae and cyanobacteria (unspecified)[1]	EC50 (unspecified duration)	417.92	2	ECHA

1 – testing read across from potassium acetate

Chronic Studies

No chronic data are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium acetate is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Bioaccumulation of sodium acetate is not expected to occur because the substance dissociates completely in aqueous media to acetate and its sodium ion. Both ions are ubiquitous in the environment. Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways. The log K_{ow} for sodium acetate is -3.72. Thus, sodium acetate does not meet the screening criteria for bioaccumulation.

The acute toxicity values for tested species are all > 1mg/L. Thus, sodium acetate does not meet the screening criteria for toxicity.

There are no chronic toxicity studies on sodium acetate. The acute E(L)C_{50} values were greater than 1 mg/L. Thus, sodium acetate does not meet the criteria for toxicity.

The overall conclusion is that sodium acetate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium acetate

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium acetate	127-09-3	Not a PBT	No	No	No	No	No	No	1	No data available	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy (DoEE). 2017b. Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

DoEE. 2017a. Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

NICNAS. 2017. Chemicals of low concern for human health based on an initial assessment of hazards, Project report prepared by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry

kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

SODIUM ACID PYROPHOSPHATE

This dossier on sodium acid pyrophosphate presents the most critical studies pertinent to the risk assessment of these substances in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium acid pyrophosphate is classified as a **tier 1** chemicals and requires a hazard assessment only.

1 BACKGROUND

Sodium acid pyrophosphate is an inorganic salt. It is widely used in food processing and in the United States, it is classified as generally recognized as safe (GRAS) for food use. In petroleum production, it can be used as a dispersant in oil well drilling muds.

Sodium acid pyrophosphate dissociates completely in aqueous media to sodium ions (Na^+) and pyrophosphate ions ($P_2O_7^{4-}$). The pyrophosphate anion is unstable in aqueous solution and hydrolyses into inorganic phosphate. Both sodium ions (Na^+) and phosphate ions (HPO_4^{2-}) are ubiquitous in the environment. Both ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Neither sodium acid pyrophosphate nor its dissociated ions are expected to bioaccumulate. Sodium acid pyrophosphate is expected to be of low toxicity concern to aquatic organisms based on a similar compound.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): disodium dihydrogen (phosphonatooxy) phosphonate

CAS RN: 7758-16-9

Molecular formula: $H_2Na_2O_7P_2$

Molecular weight: 221.94 g/mol

Synonyms: Disodium diphosphate, Disodium pytophosphate, Disodium dihydrogen pyrophosphate, Sodium acid pyrophosphate, Sodium polyphosphate, Polyphosphoric acids, sodium salts, Disodium acid pyrophosphate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of sodium acid pyrophosphate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	white solid	1	ECHA

Property	Value	Klimisch score	Reference
Melting Point	> 450 °C (pressure not provided)	1	ECHA
Boiling Point	No data as the substance is a solid which melts above 300°C	-	ECHA
Density	2630 kg/m^3 @ 22°C	1	ECHA
Vapour Pressure	0 Pa @ 20 °C	1	ECHA-
Partition Coefficient (log K_{ow})	No data as the substance is a solid inorganic	-	ECHA
Water Solubility	170 g/l @ 20 °C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium acid pyrophosphate.

NICNAS has assessed sodium acid pyrophosphate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

As an inorganic substance, sodium acid pyrophosphate is expected to disassociate completely in aqueous media to sodium ions (Na^+) and pyrophosphate ions ($P_2O_7^{4-}$). The pyrophosphate anion is unstable in aqueous solution and hydrolyses into inorganic phosphate:

$P_2O_7^{4-} + H_2O \rightarrow 2HPO_4^{2-}$.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7758-16-9%2C+

Both (Na^+) and phosphate ions (HPO_4^{2-}) are ubiquitous in the environment. Both ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated (Ganong, 1995). Neither sodium acid pyrophosphate nor its dissociated ions are expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium acid pyrophosphate is of low toxicity concern to aquatic and terrestrial organisms. Details are provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sodium acid pyrophosphate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Acid Pyrophosphate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Freshwater fish	96-hour LC_{50}	100 mg/L[1]	1	ECHA
Daphnia magna	48-hour EC_{50}	100 mg/L[1]	1	ECHA
Desmodesmus subspicatus	72 hour EC_{10}	100 mg/L[1]	1	ECHA

1 – based on read across to phosphoric acid, potassium salt (2:3), dihydrate (CAS No. 66922-99-4)

Chronic Studies

No chronic studies were identified.

C. Terrestrial Toxicity

Table 4 lists the results of terrestrial toxicity studies conducted on sodium acid pyrophosphate.

Table 4 Terrestrial Toxicity Studies on Sodium acid pyrophosphate*

Test Species	Endpoint	Results (mg/kg soil dw)	Klimisch score	Reference
Eisenia foetida	14-day LC_{50}	> 3,500	2	ECHA

*Study used test material potassium hydrogen phosphate (CAS No. 7778-77-0)

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium acid pyrophosphate is an inorganic salt that dissociates to its respective cations and anions in aqueous solutions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistence criteria are not considered applicable to this inorganic salt.

Sodium and phosphate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Therefore, sodium acid pyrophosphate is not expected to bioaccumulate.

Both chronic and acute aquatic toxicity data are >1 mg/L. Thus, sodium acid pyrophosphate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium acid pyrophosphate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium acid pyrophosphate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium acid pyrophosphate	7758-16-9	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

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Ganong, W.F. (1995). Review of Medical Physiology, 17th Edition, Appleton & Lange, Norwalk, Connecticut, USA.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic

PEC	Predicted exposure concentrations
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SODIUM BICARBONATE

This dossier on sodium bicarbonate presents the most critical studies pertinent to the risk assessment of sodium bicarbonate in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium bicarbonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Due to its high water solubility and low vapour pressure, sodium bicarbonate will be found predominantly in the aquatic environment where it dissociates completely to sodium (Na+) and bicarbonate (HCO_3^-) ions. Both ions are ubiquitous in the environment. Sodium bicarbonate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium; hydrogen carbonate

CAS RN: 144-55-8

Molecular formula: $CH_2O_3.Na$

Molecular weight: 84.01 g/mol

Synonyms: Sodium bicarbonate; sodium hydrogen carbonate; baking soda; carbonic acid monosodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Bicarbonate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	-	PubChem
Melting Point	Decomposes @ 50°C (pressure not provided)	-	PubChem
Boiling Point	-	-	-
Density	2,100 kg/m^3 (temperature not indicated)	-	PubChem

Property	Value	Klimisch score	Reference
Vapour Pressure	Negligible, ionizable inorganic compound	-	OECD, 2002
Partition Coefficient (log K_{ow})	Not relevant, ionizable inorganic compound	-	OECD, 2002
Water Solubility	100 g/L @ 25°C	-	PubChem
Dissociation Constant (pKa)	6.3 (temperature not indicated)	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium bicarbonate.

NICNAS has assessed Portland cement in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] . In addition, based on an assessment of environmental hazards, NICNAS also identified sodium bicarbonate as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Due to its high water solubility and negligible vapour pressure, sodium bicarbonate will be found predominantly in the aquatic environment where it dissociates completely to sodium (Na^+) and bicarbonate (HCO_3^-) ions. Both ions are ubiquitous in the environment (UNEP, 1995).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=144-55-8

When bicarbonate is dissolved in water, a re-equilibration takes place according to the following equations:

$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ pKa=10.33

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ pKa = 6.35

Only a small fraction of the dissolved CO_2 is present as H_2CO_3 (carbonic acid), the major part is present as CO_2. The amount of CO_2 in water is in equilibrium with the partial pressure of CO_2 in the atmosphere. The CO_2/ HCO_3^-/ CO_3^{2-} equilibria are the major buffer of the pH of freshwater.

Based on the above equations, CO_2 is the predominant species at a pH smaller than 6.35, while HCO_3^- is the predominant species at a pH in the range of 6.35-10.33 and CO_3^{2-} is the predominant species at a pH higher than 10.33.

Geochemical and biological processes dictate the natural concentration of CO_2/ HCO_3^-/ CO_3^2 in freshwater. For instance, a continuous source of carbonate in freshwater is from the deposition of carbonate ions from the dissolution of minerals. Carbon dioxide comes from the decay of organic matter in aquatic ecosystems. On the other hand, carbon dioxide dissolved in freshwater is utilised by plants in photosynthesis.

The addition of sodium bicarbonate to the aquatic environment could potentially increase the sodium and bicarbonate concentration. However, unlike sodium carbonate, sodium bicarbonate does not increase the pH of the water to high and/or lethal levels. Addition of bicarbonate to water will move the pH towards 8.34 (the mean of the two pKa values from the two above equations) (OECD, 2002).

Na^+ and HCO_3^- ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium bicarbonate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on sodium bicarbonate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Bicarbonate

Test Species	Endpoint	Results (g/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	7,700	2	OECD, 2002

Test Species	Endpoint	Results (g/L)	Klimisch score	Reference
Lepomis macrochirus	96-hour LC_{50}	7,100	2	OECD, 2002
Daphnia magna	48-hour EC_{50}	4,100	2	OECD, 2002
Daphnia magna	48-hour EC_{50}	>1,000	2	OECD, 2002
Ceriodaphnia dubia	48-hour EC_{50}	1,020	2	OECD, 2002

Chronic Studies

The NOEC from a 21-day *Daphnia* reproduction study is >576 mg/L (OECD, 2002) [Kl. score = 2].

C. Terrestrial Toxicity

The 48-hour LC_{50} and NOEC from an acute honeybee test on sodium bicarbonate was >24 and 24 µg/bee, respectively (OECD, 2002).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium bicarbonate is an inorganic salt that dissociates completely to sodium and bicarbonate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and bicarbonate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria is not considered applicable to this inorganic salt.

Sodium and bicarbonate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Therefore, sodium bicarbonate is not expected to bioaccumulate and does not meet the screening criteria for bioaccumulation.

The NOEC for sodium bicarbonate from a chronic *Daphnia* study is >0.1 mg/L. The acute EC_{50} values for sodium bicarbonate are >1 mg/L in fish and invertebrates. Thus, sodium bicarbonate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium bicarbonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium bicarbonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Bicarbonate	144-55-8	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

NICNAS. (2017). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Uniong/L grams per litre
IUPAC	International Union of Pure and Applied Chemistry
Kl	Klimisch scoring system

kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
µg	micrograms

SODIUM CARBONATE

This dossier on sodium carbonate presents the most critical studies pertinent to the risk assessment of sodium carbonate in its use in drilling muds and water treatment systems. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on sodium carbonate (OECD, 2002a,b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium carbonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Due to its high water solubility and low vapour pressure, sodium carbonate will be found predominantly in the aquatic environment where it dissociates completely to sodium (Na+) and carbonate (CO_3^{2-}) ions. Both ions are ubiquitous in the environment. Na+ and CO_3^{2-} ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. Sodium carbonate is of low toxicity concern to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): disodium carbonate

CAS RN: 497-19-8

Molecular formula: $CH_2O_3.2Na$

Molecular weight: 106 g/mol

Synonyms: sodium carbonate; disodium carbonate; carbonic acid, disodium salt; bisodium carbonate; soda ash, calcined soda

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Sodium Carbonate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid; white powder	1	ECHA
Melting Point	851°C @ 101.3 kPa	2	ECHA
Boiling Point	Decomposes	-	ECHA
Density	2520 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	Negligible	-	ECHA
Partition Coefficient (log K_{ow})	Not relevant, ionizable inorganic compound	-	ECHA
Water Solubility	212.5 g/L @ 20°C	2	ECHA

Property	Value	Klimisch score	Reference
Dissociation constant (pKa)	10.33 @ 20°C	2	ECHA

Aqueous solutions are strongly alkaline. At 25°C, the pH of 1, 5 and 10 wt% sodium carbonate solutions are 11.37, 11.58 and 11.70, respectively (Eggeman, 2001).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium carbonate.

NICNAS has assessed sodium carbonate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Due to its high water solubility and negligible vapour pressure, sodium carbonate will be found predominantly in the aquatic environment where it dissociates completely to sodium (Na^+) and carbonate (CO_3^{2-}) ions. Both ions are ubiquitous in the environment (UNEP, 1995).

Addition of sodium carbonate to an aquatic ecosystem will result in an increase in alkalinity and a tendency to increase the pH. The carbonate ions will react with water, forming bicarbonate (HCO_3^-) and hydroxide (OH^-) ions until an equilibrium is reached. A re-equilibration takes place when carbonate (CO_3^{2-}) is dissolved in water according to the following equations:

$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ pKa=10.33

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ pKa = 6.35

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=497-19-8

Only a small fraction of the dissolved CO_2 is present as H_2CO_3 (carbonic acid), the major part is present as CO_2. The amount of CO_2 in water is in equilibrium with the partial pressure of CO_2 in the atmosphere. The CO_2/ HCO_3^-/ CO_3^{2-} equilibria are the major buffer of the pH of freshwater.

Based on the above equations, CO_2 is the predominant species at a pH smaller than 6.35, while HCO_3^- is the predominant species at a pH in the range of 6.35-10.33 and CO_3^{2-} is the predominant species at a pH higher than 10.33.

A release of sodium carbonate into the aquatic environment from the use of sodium carbonate could potentially increase the sodium concentration and the pH in the aquatic environment. Table 3 shows the concentration of sodium carbonate needed to increase the pH to values of 9.0, 10.0 and 11.0.

Table 3 Sodium Carbonate Concentration (mg/L) Needed to Increase pH (DeGroot et al., 2002; taken from OECD, 2002b)

Buffer capacity*	Final pH**		
	9.0	10.0	11.0
0 mg/L HCO_3^- (distilled water)	11.1 (0.6)	16 (6.1)	603 (61)
20 mg/L HCO_3^- (10^{th} percentile of 77 rivers)	2.7 (21)	32 (26)	766 (81)
106 mg/L HCO_3^- (mean value of 77 rivers)	9.7 (107)	102 (112)	1467 (167)
195 mg/L HCO_3^- (90^{th} percentile of 77 rivers)	17 (196)	175 (201)	2192 (256)

*The initial pH of a bicarbonate solution with a concentration of 20-195 mg/L is 8.3 (calculated).
**The final concentration of bicarbonate is given in parentheses.

Na^+ and CO_3^{2-} ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues (OECD, 2002b).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium carbonate is of low toxicity concern to aquatic and terrestrial organisms.

B. Aquatic Toxicity

Acute Studies

The results of the aquatic toxicity studies conducted on sodium carbonate are presented in Table 4.

Table 4 Aquatic Toxicity Studies on Sodium Carbonate (OECD, 2002a,b)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Bluegill sunfish	96-hour LC_{50}	300	2	OECD, 2002a,b

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Mosquitofish	96-hour LC_{50}	740	2	OECD, 2002a,b
Bluefill sunfish	24-hour LC_{50}	385	4	OECD, 2002a,b
Molly	50-hour LC_{50}	297	4	OECD, 2002a,b
Ceriodaphnia dubia	48-hour EC_{50}	200 - 227	2	OECD, 2002a,b

There are other studies conducted on invertebrates, but the results of these studies were not included in Table 4 because of the low reliability of the data (OECD, 2002a,b). No studies on algae were identified (OECD, 2002a,b).

C. Terrestrial Toxicity

No studies were identified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium carbonate is an inorganic salt that dissociates completely to sodium and carbonate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and carbonate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Sodium and carbonate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Thus, sodium carbonate is not expected to bioaccumulate and does not meet the screening criteria for bioaccumulation.

No chronic aquatic toxicity data exist on sodium carbonate; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Therefore, sodium carbonate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium carbonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium carbonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium carbonate	497-19-8	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g	gram

GLP	good laboratory practice
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
m	metre
mg/L	milligram per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
wt%	weight percent

SODIUM CARBOXYMETHYLCELLULOSE

This dossier on sodium carboxymethylcellulose presents the most critical studies pertinent to the risk assessment of sodium carboxymethylcellulose in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium carboxymethylcellulose is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium carboxymethylcellulose (Na CMC) is a white or slightly yellowish powder. It is biodegradable, but not readily biodegradable, and it is not expected to bioaccumulate. Sodium carboxymethylcellulose is a low concern for toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): sodium;2,3,4,5,6-pentahydroxyhexanal;acetate

CAS RN: 9004-32-4

Molecular formula: $C_8H_{15}NaO_8$

Molecular weight : 262 g/mol (for monosubstituted structural unit); variable 21,000 g/mol – 500,000 g/mol (for macromolecules)

Synonyms: Sodium carboxymethylcellulose, Carboxymethylcellulose, sodium; cellulose, carboxymethyl ether, sodium salt; sodium CMC; sodium cellulose glycolate; sodium CMC; Na CMC

3 PHYSICO-CHEMICAL PROPERTIES

Sodium carboxymethylcellulose is a white or slightly yellowish, almost odourless and tasteless hydroscopic powder, consisting of very fine particles, fine granules or fine fibres (WHO, 1967).

Sodium carboxymethylcellulose, one of major cellulosic ethers, is widely used as a binding, thickening and stabilising agent (Lee et al. 2018).

Pharmaceutical grades of sodium carboxymethylcellulose are available commercially at degree of substitution (DS) values of 0.7, 0.9, and 1.2, with a corresponding sodium content of 6.5%–12% wt. It is also available in several different viscosity grades. Sodium carboxymethylcellulose is highly soluble in water at all temperatures, forming clear solutions. Its solubility depends on its degree of substitution (Düring et al, 2019).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium carboxymethylcellulose.

NICNAS has assessed sodium carboxymethylcellulose in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium carboxymethylcellulose is biodegradable, but is not considered to be readily biodegradable. It is not expected to bioaccumulate.

B. Partitioning

All of the polymers in this group are expected to be water soluble. If discharged into natural waters, sodium carboxymethylcellulose is expected to be present as a polyanion as a result of the ionisation of the carboxymethyl substituents. Comparatively complex partitioning behaviour in aquatic systems may occur based on the well-established interactions between colloids and carboxymethylcellulose, which is a key part of the function of this polymer in laundry detergents (de Oude 1992).

C. Biodegradation

In an OECD 301A test, sodium carboxymethylcellulose (DS 0.7) showed 25% biodegradation after 28 days, followed by a much slower increase of the biodegradation percentage. At day 110, 58% of the theoretical oxygen demand (ThOD) was consumed, leading the investigators to conclude that there was complete degradation of sodium carboxymethylcellulose (VanGinkel and Gayton, 1996). Therefore, sodium carboxymethylcellulose is degradable, but not readily biodegradable. [Kl. score = 1]

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9004-32-4

In an OECD 302A test, only 50% of the carbon from sodium carboxymethylcellulose (DS 0.7) was removed (VanGinkel and Gayton, 1996).

Other studies have also shown partial degradation of sodium carboxymethylcellulose in ready and inherent biodegradability tests (reviewed in VanGinkel and Gayton, 1996). [Kl. score = 4]

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental partition coefficient data are available for sodium carboxymethylcellulose. Based on its high water solubility, the substance is likely to be mobile in the environment.

E. Bioaccumulation

Sodium carboxymethylcellulose is a water-soluble semisynthetic polymer with a high molecular weight (approximately 21,000 to 500,000 daltons). Due to its large molecular weight, it is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium carboxymethylcellulose is a low concern for toxicity to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 2 lists the results of acute aquatic toxicity studies conducted on sodium carboxymethylcellulose.

Table 2 Acute Aquatic Toxicity Studies on sodium carboxymethylcellulose or sodium carboxymethylcellulose

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachydanio rerio	96-hour LC_{50}	>2,500*	1	VanGinkel and Gayton (1996)
Daphnia magna	48-hour EC_{50}	>5,000*	1	VanGinkel and Gayton (1996)
Daphnia magna	48-hour EC_{50}	87.26**	2	Warne and Schifko (1999)
Selenastrum capricornutum	96-hour EC_{50}	500*	1	VanGinkel and Gayton (1996)

*sodium carboxymethylcellulose (0.7) was tested.
** sodium carboxymethylcellulose was tested.

Additional aquatic toxicity studies on sodium carboxymethylcellulose by Schöberl *et al.* (1988) reported LC_0 values of >250 to 1,000 mg/L for fish and >1,000 mg/L for *Daphnia*.

VanGinkel and Gayton (1996) also tested the degradation products of sodium carboxymethylcellulose from *Agrobaceterium* CM-1 in acute toxicity studies. There was no toxicity to

Brachydanio rerio (1,000 mg/L), *Daphnia magna* (1,000 mg/L) or *Selenastrum capricornutum* (500 mg/L).

It is unclear why there is a large difference in *Daphnia* EC_{50} values between the studies of VanGinkel and Gayton (1996) and Warne and Schifko (1999). One possibility is that the two laboratories may have tested different sodium carboxymethylcellulose products. VanGinkel and Gayton (1996) tested sodium carboxymethylcellulose (0.7), whereas Warne and Schifko (1999) tested sodium carboxymethylcellulose (with no further description) in their study. However, the studies by Schöberl et al. (1988) reported an acute toxicity for *Daphnia* that is similar to that reported by VanGinkel and Gayton (1996). As a water-soluble polymer, sodium carboxymethylcellulose or sodium carboxymethylcellulose would be expected to exhibit low toxicity due to its large molecular weight and its inert characteristics.

Chronic Studies

No additional studies were identified. However, VanGinkel and Gayton (1996) reported that there was no toxicity to *Daphnia* in a 21-day reproduction test when tested using effluent from sodium carboxymethylcellulose treated with in a conventional activated sludge system (CAS system), (*i.e.*, no toxicity due to partial degradation of sodium carboxymethylcellulose).

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium carboxymethylcellulose is a water-soluble semisynthetic polymer that is not readily biodegradable. Therefore, it meets the screening criteria for persistence.

Sodium carboxymethylcellulose is a water-soluble semisynthetic polymer that has a high molecular weight (approximately 21,000 to 500,000 daltons) which limits its bioavailability to aquatic organisms. Therefore, it is not expected to bioaccumulate and does not meet the screening criteria for bioaccumulation.

The acute EC_{50} of sodium carboxymethylcellulose is >1 mg/L in fish, invertebrates and algae. Therefore, it does not meet the screening criteria for toxicity.

The overall conclusion is that sodium carboxymethylcellulose is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium carboxymethylcellulose.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Carboxymethylcellulose	9004-32-4	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
CAS system	conventional activated sludge system

CMC	carboxymethylcellulose
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DS	degree of substitution
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	theoretical oxygen demand
WHO	World Health Organization

SODIUM CHLORIDE

This dossier on sodium chloride presents the most critical studies pertinent to the risk assessment of sodium chloride in its use in drilling muds and hydraulic fracturing fluids and as a cement additive chemical. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium chloride is a naturally occurring inorganic complex. It is not of substantial toxicological concern nor is it particularly harmful to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): sodium; chloride

CAS RN: 7647-14-5

Molecular formula: NaCl

Molecular weight: 58.44 g/mol

Synonyms: Halite, Salt, Table salt, Saline, Rock salt, Common salt, Dendritis, Purex

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of SODIUM CHLORIDE

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White crystaline solid	-	ECHA
Melting Point	801 °C @ 101.3 kPa	-	ECHA
Boiling Point	The study does not need to be conducted, because NaCl is a solid which melts above 300°C.	1	ECHA
Density	2163 kg/m^3 @ 20 °C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	The study does not need to be conducted, because NaCl is a solid which melts above 300°C	1	ECHA
Partition Coefficient (log K_{ow})	The study does not need to be conducted, because NaCl is inorganic	1	ECHA
Water Solubility	317 g/L @ 20°C	2	ECHA
Dissociation Constant (pKa)	Not applicable, NaCl is an electrovalent substance	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium chloride.

NICNAS has assessed sodium chloride in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium chloride (NaCl) dissociates completely in aqueous solutions to sodium (Na^+) and chloride (Cl^-) ions. Sodium chloride and its dissociated ions are ubiquitous in the environment.

The transport and/or leaching of sodium (Na^+) and chloride (Cl^-) ions is affected by clay minerals (type and content), pH, and organic matter. Similar to potassium, sodium ions are less mobile and

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7647-14-5

less prone to leaching than anions in soil, such as chloride and nitrate (NO_3^-). Chloride binds only weakly to soil particles, and therefore follows water movement (DoEE, 2017; OECD, 2001).

Chloride (Cl^-) ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated (OECD, 2001). Neither sodium chloride nor its dissociated ions are expected to bioaccumulate.

Release to surface waters under the assessed circumstances is expected to have limited long-term environmental effects as these salts are ubiquitous and are present in most water, soil and sediment, therefore organisms are adapted to a level of exposure. The magnitude of the acute effect for a receiving aquatic environment would depend on the released concentrations as well as the degree of adaptation of species present to these naturally occurring ions and salts (DoEE, 2017).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium chloride is of low acute toxicity concern to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion.

B. Aquatic Toxicity

Acute Studies: The 96-hour LC_{50} value of 5,840 mg/L for sodium chloride was determined in a continuous flow-through exposure system with bluegill sunfish (*Lepomis macrochirus*) (ECHA) [Kl. Score =1].

The EC_{50} 48-hour (*Daphnia magna immobilisatoin*) was determined to be 1,900 mg/L (ECHA) [Kl. Score = 2].

The EC_{50} of NaCl at 96 hours to *Lemna* was determined for comparison and found to be 6,870 mg/L (6.87 g/L) (ECHA) [Kl. Score = 1].

Chronic Studies

The 33-day NOEC value of 252 mg/L for sodium chloride was determined in a continuous flow-through exposure system with early life stage fathead minnows (*Pimephales promelas*) (ECHA) [Kl. Score = 2].

A 21-day NOEC (reproduction, *Daphnia pulex*) was determined to be 314 mg/L (ECHA) [Kl. Score = 2].

C. Terrestrial Toxicity

The mean 14-day LC_{50} for three experiments conducted with the earthworm, *E. fetida* was 3,296 mg NaCl/kg soil dw. The 10-week NOEC (based on mortality) was 3,507 mg NaCl/kg soil for the earthworm, *E. fetida* (ECHA) [Kl. Score = 2].

In a 7-day exposure study with red fescue grass, the EC_{50} for germination was 500.8 mg NaCl/kg soil dw. In a 7-day exposure study with Kentucky bluegrass the NOEC for stem growth was 243 mg NaCl/kg soil dw (ECHA) [Kl. Score = 2].

The 12-hour LD_{50} for wild house sparrows was approximately 3,000 - 3,500 mg/kg NaCl (ECHA) [Kl. Score = 2].

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium chloride is an inorganic mineral. Thus, biodegradation is not applicable to this substance. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to sodium chloride.

Bioaccumulation in fish is not expected given the inorganic nature of the substance. Thus, sodium chloride does not meet the screening criteria for bioaccumulation.

The NOECs from the acute aquatic toxicity studies on sodium chloride are greater than 1 mg/L, thus sodium chloride, does not meet the criteria for toxicity.

Sodium chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium chloride.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium chloride	7647-14-5	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment and Energy [DoEE]. (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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OECD. (2001). Screening Information Assessment Report (SIAR) for Potassium chloride (CAS No. 7447-40-7), UNEP Publications. Available at: https://hpvchemicals.oecd.org/UI/SIDS_Details.aspx?id=68BF142A-D550-432C-8C48-13883944BA1D.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IC	growth inhibition concentration

IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
LD	lethal dose
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SODIUM DODECYL SULPHATE

This dossier on sodium dodecyl sulphate (SDS) presents the most critical studies pertinent to the risk assessment of SDS in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – A review of aquatic toxicity data indicates a classification of SDS as a tier 2 substance based on acute and chronic aquatic toxicity for invertebrates. However, the substance has been determined to rapidly biodegrade in the environment and the decomposed by-products are benign. As a result, SDS is classified overall as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

SDS is mainly used in detergents for laundry with many cleaning applications. It is a highly effective surfactant and is used in any task requiring the removal of oily stains and residues; for example, it is found in higher concentrations with industrial products including engine degreasers, floor cleaners and car exterior cleaners. In lower concentrations, it is found in hand soap, toothpastes, shampoos, shaving creams and bubble bath formulations, for its ability to create a foam (lather), for its surfactant properties and in part for its thickening effect.

SDS is considered a generally recognized as safe (GRAS) ingredient for food use according to the United States Food and Drug Administration (USFDA) (21 CFR 172.822) and is often used as an emulsifying agent and whipping aid.

SDS is readily biodegradable. It is not expected to bioaccumulate. Due to its high water solubility, SDS is unlikely to adsorb to soil or sediment. Due to its rapid biodegradation, SDS will result in low toxicity to aquatic organisms under environmental conditions. The decomposed by-products of SDS are benign to the environment.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): sodium dodecyl sulfate

CAS RN: 151-21-3

Molecular formula: $C_{12}H_{25}NaO_4S$

Molecular weight: 288.38 g/mol

Synonyms: Irium, Lauryl Sulfate, Sodium, Sodium Lauryl Sulfate, Sulfate, Sodium Dodecyl, Sulfate, Sodium Lauryl

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of SDS

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, granular solid at ambient temperature.	1	ECHA
Melting Point	205°C (pressure not provided)	2	ECHA
Boiling Point	216 °C @102.2 kPa	1	ECHA
Density	630 kg/m^3	1	ECHA
Vapour Pressure	≤ 0.18 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	≤ -2.03 @ 20°C	1	ECHA
Water Solubility	> 130 g/L @ 20°C	1	ECHA
Dissociation Constant (pKa)	1.31 @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for SDS.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

SDS readily biodegradable. It has a very low sorption potential and is not expected to bioaccumulate.

B. Partitioning

SDS is highly soluble in water. Volatilization from water or moist soil surfaces is not expected to be an important fate process based upon its water solubility and that it is a salt. It is not expected to volatilize from dry soil surfaces based upon its estimated vapour pressure.

Hydrolysis is not expected to be an important environmental fate process since this compound lacks of functional groups that hydrolyze under environmental conditions (ph 5 to 9).

C. Biodegradation

All substances in the alkyl sulfate category were found to be readily biodegradable.

The ready biodegradability of C12AS Na salts was tested in two aerobic studies. After 10 days of exposure, 81.5% of the test substance was already degraded; after 28 days, 95% of the test substance was mineralised. Therefore, the test substance is readily biodegradable according to OECD criteria (ECHA).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

SDS is indicated to be of low sorption potential with an estimated K_{oc} value of 316 to 446, which corresponds to log K_{oc} values in the range of 2.50 to 2.65 (ECHA). Based on this K_{oc} value, if released to soil, SDS is expected to have moderate mobility. If released into water, based on its high water solubility and low vapour pressure, SDS to preferentially partition to the water column.

E. Bioaccumulation

In accordance with column 2 of Annex IX 9.3.2 of REACH Regulation EC 1907/2006 (ECHA), bioaccumulation testing in aquatic species is not required as the substance has a low potential for bioaccumulation (log K_{ow} of < 3).

The log K_{ow} for SDS is $\leq$ -2.03. Thus, SDS is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

SDS is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Due to its rapid biodegradation, SDS will result in low toxicity to aquatic organisms under environmental conditions. The biodegradation of SDS occurs via hydrolytic cleavage of the sulfate ester bond leaving inorganic sulfate and fatty alcohol. These fatty alcohols undergo oxidation to produce fatty acids, which are degraded by β-oxidation and fully mineralized and incorporated into the biomass. Thus, the decomposed by-products of SDS are benign to the environment (Bondi, Cara Am et al., 2015).

Acute Studies

Fish: Numerous studies are available investigating the acute toxicity of SDS to freshwater and marine fish since SDS is an economically important surfactant and was frequently used as reference substance in toxicity tests. The data set is comprised of several publications with acceptable quality and validity focusing on standard and non-standard species as well as one study report investigating the acute toxicity to the standard species Pimephales promelas. The study was performed according to OECD guideline 203. Fish were exposed in a flow-through system to five test concentrations up to 48 mg/L nominal concentration, corresponding to 40 mg/L measured concentration. Mortality of fish was evaluated every 24 hours throughout the 96-hour test period. The 96-hour LC_{50} value is determined to be 29 mg/L based on measured concentration. This study is considered to be the most reliable study since it was performed under flow-through conditions and is very well documented as the study was performed for regulatory purposes. Although this effect value is not the lowest observed in the data set, it was used for hazard assessment since (i) this study is rated as the most comprehensive and reliable one and (ii) the remaining data set is biased because for most additional species tested, several effect values are existing in the literature but always the lowest obtained value per species is listed and no averaging was performed. This was done because the data set is primarily presented to statistically assess the general susceptibility of fish to SDS in comparison to aquatic invertebrates and algae using a conservative approach. (ECHA). [Kl score = 2]

Invertebrates: Numerous studies are available investigating the acute toxicity of SDS to freshwater and marine invertebrates, since SDS is an economically important surfactant and was frequently used as reference substance in toxicity tests. The data set is comprised of several publications with acceptable quality and validity focusing on standard and non-standard species, as well as one study report investigating the acute toxicity to the standard species *Ceriodaphnia dubia*. The non-GLP study was performed equivalent to the conditions as described in OECD guideline 202. *Daphnids* were exposed in a flow-through system to six test concentrations (+ control) in the range of 0.38 to 101 mg/L. Mortality of *daphnids* was evaluated every 24 hours throughout the 48-hour test period. The 48-hour LC_{50} value is determined to be 5.5 mg/L (4.28 – 7.2 mg/L). This study is considered to be the most reliable study since it was performed under flow-through conditions, which enabled stable test substance concentrations and is well documented as the study was performed for regulatory purposes. Although this effect value is not the lowest observed in the data set it was used for hazard assessment since (i) this study is rated as the most comprehensive and reliable one and (ii) the remaining data set is biased because several effect values are existing in the literature for many additional (standard) species tested but always the lowest obtained value per species is listed and no averaging was performed. This was done because the data set is primarily presented to statistically assess the general susceptibility of aquatic invertebrates to SDS in comparison to fish and algae using a conservative approach. [Kl Score = 2]

Chronic Studies

Fish: Two studies are available investigating the long-term toxicity of SDS to freshwater fish. The key study tested the effects of the test substance in a juvenile fish growth test using *Pimephales promelas* as test organism. Juveniles were exposed over a test period of 42 days to the test substance in a flow-through system using river water. Mortality as well as growth (weight) were recorded. No adverse effects were observed after 42 days of exposure to up to the highest tested concentration of 1.36 mg/L. Thus the 42-day NOEC value is determined to be ≥ 1.36 mg/L based on measured concentrations (ECHA) [Kl Score=2].

Invertebrates: A non-GLP, 7-day reproduction toxicity test with *Ceriodaphnia dubia* performed according to EPA-600/489/001 guideline is used as key study. *Daphnids* were exposed under flow-through conditions to five test concentrations up to 8 mg/L. An analytical check of test concentrations proved that the nominal concentrations were in agreement with the measured ones. Mortality and reproduction were evaluated daily. The 7-day NOEC value for reproduction is determined to be 0.88 mg/L based on the measured concentration (ECHA) [Kl Score=2].

A non-GLP, 40-day chronic toxicity test with *Daphnia magna* was performed. The test organism was exposed to test substance concentrations up to 8 mg/L (nominal concentration) over four consecutive generations under semi-static conditions. No special guideline was followed. Offspring *daphnids* of less than 24 hours of age were collected after 10 days of exposure to the test substance and exposed for another 10 days. This procedure was repeated three times. The overall NOEC ranged from 2 to 4 mg/L based on nominal concentrations. Another long-term toxicity test with *Daphnia magna* was reported. The study was performed according to OECD Guideline 202 P under semi-static conditions (daily renewal) with analytical confirmation of the test substance concentration. The 21-day NOEC value for reproduction is determined to be 3.2 mg/L based on the measured concentration (ECHA) [Kl Score=2].

A long-term toxicity of the freshwater cladoceran species *Pseudosida ramosa* to SDS using OECD Guideline 211 was performed. SDS concentrations from 0.25 to 4 mg/L were tested under semi-static conditions. The 21-day NOEC value is determined to be 1 mg/L based on the nominal concentration (ECHA) [Kl Score=2].

The long-term toxicity of SDS on the reproduction of *Hydra attenuata* was tested in a chronic toxicity test under semi-static conditions. The budding rate (number of buds between two feedings) was measured over an exposure time of 21 days. SDS concentrations from 5.76 to 576 mg/L were tested. A NOEC value of 5.76 mg/L is determined based on the nominal concentrations (ECHA) [Kl Score=2].

C. Terrestrial Toxicity

No data are available. However, the substance exhibits an adsorption coefficient (log K_{oc}) below 5 and is readily biodegradable. Moreover, the substance is not acutely toxic in the aquatic compartment (EC/LC_{50} for fish, *Daphnia* and algae above 1 mg/L). In case of exposure to soil, the substance is expected to rapidly degrade, thus the hazard to terrestrial organisms is negligible.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

SDS has been determined to be readily biodegradable. Thus, it is not persistent.

No data are available on bioaccumulation. However, based on the low log K_{ow}, and rapid degradation rate, bioaccumulation is not expected. Thus, SDS does not meet the screening criteria for bioaccumulation.

The NOECs from the acute aquatic toxicity studies on SDS are greater than 1 mg/L. Thus SDS, does not meet the criteria for toxicity.

Therefore, SDS is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for SDS.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
SDS	151-21-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Bondi, Cara Am et al. “Human and Environmental Toxicity of Sodium Lauryl Sulfate (SLS): Evidence for Safe Use in Household Cleaning Products.” Environmental health insights vol. 9 27-32. 17 Nov. 2015, doi:10.4137/EHI.S31765

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ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
CFR	Code of Federal Regulations
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mL	grams per millilitre
GLP	good laboratory procedure
GRAS	generally recognized as safe

IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
mbar	millibar
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SDS	sodium dodecyl sulphate
SGG	Synthetic Greenhouse Gases
USFDA	United States Food and Drug Administration

SODIUM ERYTHORBATE

This dossier on sodium erythorbate presents the most critical studies pertinent to the risk assessment of these substances in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium erythorbate is classified as a **tier 1** chemicals and requires a hazard assessment only.

1 BACKGROUND

Sodium erythorbate is an ascorbic acid. It is used as an antioxidant and preservative. It is also used in coal seam gas extraction activities to prevent precipitation of metal oxides (iron control).

Sodium erythorbate is highly soluble in water and has a low potential to bind to soil or sediment. It is ultimately biodegradable and is not expected to bioaccumulate. It is of low aquatic toxicity concern.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): sodium;(2R)-2-[(1R)-1,2-dihydroxyethyl]-4-hydroxy-5-oxo-2H-furan-3-olate

CAS RN: 6381-77-7

Molecular formula: $C_6H_7NaO_6$

Molecular weight: 198.11 g/mol

Synonyms: D-araboascorbic acid, erythorbic acid, erythroascorbic acid, isoascorbic acid, isoascorbic acid, disodium salt, isoascorbic acid, monosodium salt, isoascorbic acid, sodium salt, 2,3-didehydro-3-O-sodio-D-erythro-hexono-1,4-lactone

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Erythorbate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Odorless solid	2	ECHA
Melting Point	160°C @ 101.3 kPa	1	ECHA
Boiling Point	-	-	ECHA
Density	1702 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	0 Pa @ 20°C	2	ECHA-
Partition Coefficient (log K_{ow})	-3.29 @ 25°C	2	ECHA
Water Solubility	146 g/L at 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium erythorbate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No

Convention, Protocol or other international control	Listed Yes or No?
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium erythorbate is highly soluble in water and has a low potential to bind to soil or sediment. It is ultimately biodegradable and is not expected to bioaccumulate.

B. Biodegradation

In an OECD compliant test, the degradation after the 28-day plateau was not yet visible in the degradation curve. Thus, under strict test conditions, the substance appears to be ultimately biodegradable (under the subclassification of inherent biodegradability) (ECHA) [KI Score = 2].

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for sodium erythorbate. Based on its low log K_{ow} and high water solubility values, if released to soil, sodium erythorbate is expected to have low potential for adsorption and a high potential for mobility. If released to water, it is likely to remain in water and not adsorb to sediment.

D. Bioaccumulation

There are no bioaccumulation studies on sodium erythorbate. The bioconcentration factor (BCF) was estimated to be 0.8933 based on the Arnot-Gobas method (for the upper trophic level) (USEPA 2020). Based on the estimated BCF, bioaccumulation is not expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium erythorbate exhibits low acute toxicity to aquatic organisms. Details are provided below.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 lists the results of acute aquatic toxicity studies on sodium erythorbate.

Table 3: Acute Aquatic Toxicity Studies on Sodium Erythorbate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-h LC_{50}	>100	2	ECHA
Daphnia magna	48-h EC_{50}	>100	2	ECHA
Freshwater algae[1]	72-h EC_{50}	>160	2	ECHA

[1] – species not identified in database

Chronic Studies

No chronic aquatic toxicity studies were available for sodium erythorbate.

C. Terrestrial Toxicity

No terrestrial toxicity data were available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium erythorbate appears to be ultimately biodegradable. Moreover, the probability for rapid biodegradation according to BIOWIN v4.10 is nearly unity. Thus, sodium erythorbate does not meet the screening criteria for persistence.

The estimated log BCF value for sodium erythobate calculated from the Arnot-Gobas method (upper trophic) QSAR model is 0.8933. Thus, it does not meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity data available on sodium erythorbate. The acute $E(L)C_{50}$ values > 1 mg/L. Thus, sodium erythorbate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium erythorbate not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium erythorbate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium erythorbate	6381-77-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram

mg/L	milligrams per litre
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
PEC	Predicted exposure concentrations
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SODIUM GLUCONATE

This dossier on sodium gluconate presents the most critical studies pertinent to the risk assessment of this substance in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from Organization for Economic Cooperation and Development Screening Information Dataset (OECD SIDS) (OECD, 2004). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium gluconate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium gluconate is the organic sodium salt of gluconic acid. Sodium gluconate is a chelator that forms stable complexes with various ions and ultimately prevents these ions from engaging in chemical reactions. Gluconates are naturally occurring substances that freely dissociate to the gluconate anion and its respective cations. Gluconates is used as a chelating agent in many cleaning products, industrial applications, and foodstuffs.

Sodium gluconate is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to sediment and soil. In addition to this, sodium gluconate has a low acute toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium D-gluconate

CAS RN: 527-07-1

Molecular formula: $C_6H_{11}NaO_7$

Molecular weight: 218.14g/mol

Synonyms: SODIUM GLUCONATE, Sodium D-gluconate 527-07-1, D-Gluconic acid, monosodium salt,D-Gluconic acid sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Gluconate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Dry, white, crystalline powder	-	PubChem

Property	Value	Klimisch score	Reference
Melting Point	205-209 °C (pressure not provided)	-	OECD, 2004
Boiling Point	613.1 °C (pressure not provided)	-	OECD, 2004
Density	1790 kg/m^3	-	PubChem
Vapor Pressure	Negligible @ 25 °C	-	OECD, 2004
Partition Coefficient (log K_{ow})	-5.99	-	OECD, 2004
Water Solubility	590 g/L @ 25 °C	-	OECD, 2004
Dissociation constant (pKa)	3.70	-	OECD, 2004

Sodium gluconate is the sodium salt of gluconic acid. Gluconic acid is a naturally occurring weak acid and its dissociation in water is expected to be complete.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium gluconate.

NICNAS has assessed sodium gluconate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=527-07-1

5 ENVIRONMENTAL FATE PROPERTIES

A. Summary

Sodium gluconate is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to sediment and soil.

B. Partitioning

Sodium gluconate is highly soluble in water. Volatilization from water or moist soil surfaces is not expected to be an important fate process based upon its water solubility and that it is a salt. It is not expected to volatilize from dry soil surfaces based upon its estimated negligible vapour pressure.

C. Biodegradation

Sodium gluconate is readily biodegradable under both aerobic and anaerobic conditions. In an aerobic closed bottle test of sodium gluconate, the biodegradation was 89% expressed as the Theoretical Oxygen Demand after 28 days; while under anaerobic conditions, 100% of sodium gluconate was determined as degraded after 35 days. These data demonstrate that gluconates are readily biodegradable both under aerobic and anaerobic test conditions (OECD, 2004).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for adipic acid. Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K_{oc} value from log K_{ow} is 0.0001046 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 10 L/kg. Based on these values, sodium gluconate has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

E. Bioaccumulation

Based on a log K_{ow} value of -5.99, sodium gluconate has a very low potential for bioaccumulation. This is further supported by metabolic in vivo studies showing that gluconate is readily catabolized or utilized for glucose synthesis (OECD, 2004).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium gluconate has low acute toxicity to aquatic organisms. No chronic toxicity studies have been reported.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 presents the results of acute aquatic toxicity studies conducted on Sodium gluconate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Gluconate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
*Oryzias latipes (*Fish, freshwater)	96-hr LC_{50}	>100	-	OECD, 2004
Daphnids magna (Crustacea)	24-48h NOEC	>1000	-	OECD, 2004
Selenastrum capricornutum (Algae)	24-72 h $NOEC_r$ 24-72 h E_rC_{50}	560 >1000	-	OECD, 2004

Chronic Studies

No studies reported.

C. Terrestrial Toxicity

No terrestrial toxicity data for gluconates are available. However, the demonstrated biodegradability and the low intrinsic toxicity of gluconates that was observed for aquatic organisms, data on animal toxicokinetic and metabolism (cfr. human toxicology) and their role in mammalian carbohydrate metabolism may predict also a low effect on terrestrial organisms. Therefore, no terrestrial toxicity studies would be required (OECD, 2004).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium gluconate is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The estimated log K_{ow} for sodium gluconate is -5.99. Thus, sodium gluconate does not meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on sodium gluconate. The acute $E(L)C_{50}$ values are >1 mg/L. Thus, sodium gluconate does not meet the screening criteria for toxicity.

Therefore, sodium gluconate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium gluconate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Gluconate	527-07-1	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Organization for Economic Cooperation and Development Screening Information Dataset.[OECD SIDS] (2004). Gluconic Acid and Its Derivatives. Available online: https://hpvchemicals.oecd.org/UI/handler.axd?id=b94cc5f7-de5c-4417-b6c2-f1eb4ffcdb72

PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

USEPA. (2018). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry

KOCWIN	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effect concentration
Pa	Pascal
PBT	Persistent Bioaccumulative Toxic
QSAR	quantitative structure-activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

SODIUM HYDROXIDE

This dossier on sodium hydroxide presents the most critical studies pertinent to the risk assessment of sodium hydroxide in its use in drilling muds, hydraulic fracturing fluids and water treatment systems. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the OECD-SIDS documents on sodium hydroxide (OECD, 2002a, b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium hydroxide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium hydroxide (NaOH) is a strong alkaline substance that dissociates completely in water to sodium (Na+) and hydroxyl (OH-) ions. Both ions are ubiquitous in the environment. Na+ and OH- ions will not adsorb on the particulate matter or surfaces and will not accumulate in living tissues. Sodium hydroxide dissociates completely in aqueous solutions to sodium (Na+) and hydroxyl (OH-) ions. Sodium is an essential nutrient involved in fluid and electrolyte balance and is required for normal cellular function. The hazard of NaOH for aquatic organisms is caused by the hydroxyl ion (OH-) which has the potential to increase the pH of the aquatic environment, depending on the buffering capacity.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium hydroxide

CAS RN: 1310-73-2

Molecular formula: HNaO

Molecular weight: 40 g/mol

Synonyms: Caustic soda, soda lye, NaOH

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Sodium Hydroxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid	2	Lide, 2009; ECHA
Melting Point	318°C (solid, 100%); 52°C (60% solution)	2	ECHA
Boiling Point	1,388°C @ 101.3 kPa	2	Lide, 2009; ECHA

Property	Value	Klimisch score	Reference
Density	2130 kg/m^3, 20°C (100%) 1430 kg/m^3, 20°C (40%)	2	Lide, 2009; ECHA
Vapour Pressure	1 Pa @ 513°C	2	Lide, 2009; ECHA
Partition Coefficient (log Kow)	Not applicable	-	-
Water Solubility	Very soluble (>10 g/L @ 25°C)	2	Lide, 2009; ECHA
Dissociation Constant (pKa)	14.8 @ 25°C	2	Lide, 2009; ECHA

Sodium hydroxide (NaOH) is a strong alkaline substance that dissociates completely in water to sodium (Na^+) and hydroxyl (OH^-) ions.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium hydroxide.

NICNAS has assessed sodium hydroxide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Due to its high water solubility and low vapour pressure, sodium hydroxide will be found predominantly in the aquatic environment where it dissociates completely to sodium (Na^+) and hydroxyl (OH^-) ions. Both ions are ubiquitous in the environment (UNEP, 1995).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=1310-73-2%2C+

The addition of sodium hydroxide to an aquatic ecosystem may increase the pH depending on the buffer capacity of the receiving water. In general, the buffer capacity is regulated by the equilibria between CO_2, HCO_3^- and CO_3^{2-}:

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ ($pKa_1 = 6.35$)
$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ ($pKa_2 = 10.33$)

A release of sodium hydroxide into the aquatic environment from the use of NaOH could potentially increase the sodium concentration and the pH in the aquatic environment. Table 3 shows the concentration of sodium hydroxide needed to increase the pH to values of 9.0, 10.0, 11.0 and 12.0.

Table 3 Sodium Hydroxide Concentration (mg/L) Needed to Increase pH (DeGroot et al., 2002; taken from OECD, 2002b)

Buffer capacity*	Final pH			
	9.0	10.0	11.0	12.0
0 mg/L HCO_3 (distilled water)	0.4	4.0	40	400
20 mg/L HCO_3 (10^{th} percentile of 77 rivers)	1.0	8.2	51	413
106 mg/L HCO_3^- (mean value of 77 rivers)	3.5	26	97	468
195 mg/L HCO_3^- (90^{th} percentile of 77 rivers)	6.1	45	145	525

*The initial pH of a bicarbonate solution with a concentration of 20-195 mg/L was 8.25 to 8.35.

Na^+ and OH^- ions will not adsorb on the particulate matter or surfaces and will not accumulate in living tissues (OECD, 2002b).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Aquatic Toxicity

The OECD-SIDS SIAR on NaOH states that while the toxicity of the NaOH has been assumed to be related to the hydroxyl anion, in general a pH change could influence the speciation of other chemicals and therefore increase and/or decrease toxicity of the substance.

There are no guideline studies on NaOH; the studies summarised below have Klimisch scores of 3 or 4.

Acute Fish

The 24-hour LC_{50} to *Carassius auratus* (goldfish) is 160 mg/L. At 100 mg/L, which was equivalent to a pH of 9.8, no mortality was observed. The 48-hour LC_{50} to *Leuciscus idus melanotus*, is 189 mg/L. The 96-hour LC_{50} of *Gambusia affinis* (mosquitofish) is 125 mg/L. At 84 mg/L, no effects on the fish were observed. The pH was 9 at 100 mg/L.

Acute Invertebrate

The 48-hour LC_{50} is 40 mg/L for *Ceriodaphnia cf. dubia*. The toxicity threshold concentration of NaOH for *Daphnia magna* was reported to range from 40 to 240 mg/L.

Acute Algae

No studies were identified.

B. Terrestrial Toxicity

No studies were identified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium hydroxide is an inorganic salt that dissociates completely to sodium and hydroxide ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and hydroxide ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Sodium and hydroxide ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Thus, sodium hydroxide is not expected to bioaccumulate and does not meet the screening criteria for bioaccumulation.

No chronic toxicity data exist on sodium hydroxide; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Thus, sodium hydroxide does not meet the screening criteria for toxicity.

The overall conclusion is that sodium hydroxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium hydroxide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Hydroxide	1310-73-2	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

De Groot et al. (2002). The addition of sodium hydroxide to a solution with sodium bicarbonate to a fixed pH. Solvay Pharmaceuticals Int. Doc. No. 8320/47/01; cited in OECD, 2002a,b.

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A. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry

kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SIAR	SIDS Initial Assessment Report
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

SODIUM IODIDE

This dossier on sodium iodide presents the most critical studies pertinent to the risk assessment of sodium iodide in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – sodium iodide is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium iodide is a metal iodide salt with a Na(+) counterion. It is an inorganic sodium salt and an iodide salt. Biodegradation is not applicable to inorganic compounds and bioaccumulation is not expected. Sodium iodide is of low toxicity concern to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium iodide

CAS RN: 7681-82-5

Molecular formula: NaI

Molecular weight: 149.89 g/mol

Synonyms: Ioduril, Sodium iodide (NaI), Natriumiodid

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Sodium Iodide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White odorless crystalline solid	1	ECHA
Melting point	659°C @ 101.3 kPa	1	ECHA
Boiling point	1,304°C @ 101.3 kPa	2	ECHA
Density	3.5 g/cm^3 @ 25°C	1	ECHA
Vapor pressure	133.32 Pa @ 767°C	2	ECHA
Partition coefficient (log K_{ow})	-1.301 @ 25°C	1	ECHA

Property	Value	Klimisch score	Reference
Water solubility	165 g/L @ 25°C	1	ECHA
Dissociation Constant (pKa)	0.067 @ 25°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium iodide.

NICNAS has assessed sodium iodide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium iodide dissociates in aqueous media to sodium (Na+) and iodide (I-) ions. Biodegradation is not applicable to inorganic compounds. There are no bioaccumulation studies on sodium iodide. The low Log K_{ow} (-1.301) suggests sodium iodide will not bioaccumulate to a substantial degree ((ECHA)[Kl Score = 1]. Further, both ions are essential to living. Sodium (Na+) ions are essential to all living organisms, and its intracellular and extracellular concentrations are actively regulated (Ganong, 1995). Iodine is essential for thyroid hormone synthesis in vertebrate species. Ingested iodine is converted to iodide (I-) and absorbed. The minimum daily iodine intake that will maintain normal thyroid function is 150 mg in adult humans (Ganong, 1995).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7681-82-5%2C+

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium iodide is of low toxicity concern to aquatic organisms.

A. Aquatic Toxicity

Acute Studies

Table 1 lists the results of acute aquatic toxicity studies on sodium iodide.

Table 1 Acute Aquatic Toxicity Studies on Sodium Iodide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hr LC_{50}	>100	2	ECHA
Daphnia magna	48-hr EC_{50}	0.17[1]	2	ECHA

1 – this value is questionable since the acute value is approximately two to three orders of magnitude lower than chronic data for the same species (see below). Furthermore, acute testing conducted on a similar substance (potassium iodide) for the same species yielded a 48-hr EC50 of 7.5 mg/L (ECHA)[Kl Score = 2].

Chronic Studies

Based on the prediction done using ECOSAR version, the long term toxicity on fish was predicted for test substance. On the basis of no effects observed in a freshwater system, the NOEC value for the substance is estimated to be 66.356 mg/l for fish for 28 days of exposure duration (ECHA) [Kl. Score =2].

The 21-day NOEC in a Daphnia reproduction test is 91 mg/L (ECHA) [Kl. score = 2]. In another Daphnia reproduction test, the 21-day NOEC was 14 mg/L (ECHA) [Kl. score = 2].

The 8-day LOEC to green algae Scenedesmus quadricauda was 2,370 mg/L (ECHA) [Kl. score = 2].

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium iodide dissociates completely to sodium and iodide ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistence criteria is not considered applicable.

The low Log K_{ow} (-1.301) suggests sodium iodide will not bioaccumulate to a substantial degree. In addition, sodium ions are essential all living organisms and its intracellular and extracellular concentrations are actively regulated. The iodide ion is essential for thyroid function which is found in all vertebrates. Thus, sodium iodide does not meet the screening criteria for bioaccumulation.

The lowest NOEC value on sodium iodide is >0.1 mg/L for invertebrates and algae. While the the lowest acute E(L)C50 value is <1 mg/L for the same species of invertebrates on which acute testing was performed, this value must be questioned since it is orders of magnitude lower than chronic test data. For the purposes of this assessment, sodium iodide is not considered to be meet the criteria for toxicity.

Therefore, sodium iodide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium iodide.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium iodide	7681-82-5	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). The low value for a single acute toxicity test is not consistent with results from chronic testing for the same species. Thus, the acute test data for D. magna is not considered appropriate for use in tiered classification.

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

SODIUM LAURYL POLYOXYETHYLENE ETHER SULFATE

This dossier on sodium lauryl poloxyethylene ether sulfate presents the most critical studies pertinent to the risk assessment of this chemical in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Limited information is available for sodium lauryl poloxyethylene ether sulfate, and as a result sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES) has been selected as a surrogate chemical for this review. Based on this read-across data, sodium lauryl poloxyethylene ether sulfate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium lauryl polyoxyethylene ether sulfate is an anionic surfactant detergent. The chemicals in this group are structurally related salts of sulfated ethoxylated lauryl alcohol. Sodium lauryl polyoxyethylene ether sulfate (also known as sodium laureth sulfate), CAS No. 9004-82-4, is a generic CAS registration number that includes the group of chemicals with CAS Nos 15826-16-1, 3088-31-1, 13150-00-0, and 66161-57-7, where they have an average of one, two, three, and 12 ethoxylate units, respectively. Chemical-specific information from group member sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES) (CAS No. 3088-31-1) was used for this review. SDES is readily biodegradable. It has a strong potential for sorption to soil and sediment. However, it is not expected to bioaccumulate. SDES is of low acute and chronic toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): sodium;2-dodecoxyethyl sulfate

CAS RN: 9004-82-4

Molecular formula: $C_{14}H_{29}NaO_5S$

Molecular weight: 332.43 g/mol

Synonyms: sodium lauryl polyoxyethylene ether sulfate; sodium laureth sulfate; dodecyl sodium ethoxysulfate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium 2-(2-Dodecyloxyethoxy) Ethyl Sulfate[1]

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Odourless and colourless liquid	1	ECHA
Melting Point	Not available	-	-
Boiling Point	113.4 °C @92 kPa	1	ECHA
Density	1990 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	1.33 x 10^{-10} Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	-0.602 @ 39°C	1	ECHA
Water Solubility	1000 g/L @ 39°C	1	ECHA
Dissociation Constant (pKa)	2.2 x 10^{-18} @ 20°C	1	ECHA

[1] - Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data is shown for read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (CAS No. 3088-31-1).

The chemicals in this group are structurally related salts of sulfated ethoxylated lauryl alcohol. The synthesis of the chemicals occurs through similar processes. Lauryl alcohol is ethoxylated with ethylene oxide to form a polyethoxy ether. The terminal alcohol group is then sulfated with sulfur trioxide. The product is neutralised with either sodium or ammonium hydroxide, producing the chemicals of this group. The sodium and ammonium ions are not expected to significantly affect the hazardous properties of the chemicals.

The number of ethoxylate units usually has an average value between one and four. Sodium laureth sulfate, CAS No. 9004-82-4, is a generic CAS registration number that includes the group of chemicals with CAS Nos 15826-16-1, 3088-31-1, 13150-00-0, and 66161-57-7, where they have an average of one, two, three, and 12 ethoxylate units, respectively.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium lauryl polyoxyethylene ether sulfate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No

Convention, Protocol or other international control	Listed Yes or No?
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data is shown for read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES, CAS No. 3088-31-1).

SDES is readily biodegradable. It has a strong potential for sorption to soil and sediment. However, it is not expected to bioaccumulate.

B. Partitioning

SDES is highly soluble in water. Volatilization from water or moist soil surfaces is not expected to be an important fate process based upon its water solubility and that it is an ionic compound. It is not expected to volatilize from dry soil surfaces based upon its estimated vapour pressure.

The hydrolysis rate constant of sodium 2-(2-dodecyloxyethoxy) ethyl sulfate is estimated to be $454767x10^{-11}$ cm^3/molecule-sec. at half life of 2.822 hrs. The estimated half life of the substance indicates that the substance is moderately hydrolysable (ECHA) [Kl. Score = 2].

C. Biodegradation

By applying weight of evidence approach, SDES was found to be readily biodegradable with 50% to 71.199 % percentage degradation (ECHA) [Kl. Score = 2]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for SDES. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from the molecular connectivity index (MCI) and log K_{oc} are 2,111 and 3.324 L/kg, respectively (ECHA). Based on this K_{oc} value, if released to soil, SDES is expected to strongly adsorb to soil and have a low potential for mobility. If released to water, based on the K_{oc} value and its high water solubility, it is also expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on SDES. The BCF was estimated to vary between 70.79 and 72.127 in aquatic organisms and fish (ECHA) [Kl. Score = 2]. Based on the log K_{ow} (-2.03) and the calculated BCFs, bioaccumulation is not to be expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data is shown for read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES, CAS No. 3088-31-1).

SDES is of low acute and chronic toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on SDES.

Table 3 Acute Aquatic Toxicity Studies on SDES (CAS No. 3088-31-1)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hour LC_{50}	25	2	ECHA
Danio rerio	96-hour LC_{50}	102.59	2	ECHA
Oryzias latipes	48-hour LC_{50}	46	2	ECHA
Daphnia magna	48-hour LC_{50}	86.09	2	ECHA
Pseudokirchneriella subcapitata	72-hour EC_{50} (growth rate)	115.072	2	ECHA
Laminaria hyperborea	24-hour EC_{50}	100 (cell changes)*	2	ECHA

*Data for CAS No. 9004-82-4 (SLES).

Chronic Studies

Based on the prediction done using ECOSAR version 1.1, the long term toxicity on fish was predicted for SDES. On the basis of effects observed in a static fresh water system, the NOEC value for the substance is estimated to be 36.507 mg/L for fish for 28 days of exposure duration (ECHA) [Kl. Score = 2].

Based on the prediction done using ECOSAR version 1.1, the long term toxicity on aquatic invertebrate was predicted for SDES. On the basis of effects observed in a static freshwater system, the NOEC value for the test substance is estimated to be 20.059 mg/L for aquatic invertebrate for 21 days of exposure (ECHA) [Kl. Score = 2].

Since SDES is readily biodegradable in an aquatic environment it can be concluded that the test chemical can be considered as non-toxic to fish and aquatic invertebrates at environmentally relevant concentrations (ECHA).

C. Terrestrial Toxicity

The lethal concentration (LC50) of SDES in soil macroorganism [Eisenia fetida (worms)] in a long term toxicity study of 14 days on the basis of mortality effect was estimated to be 2600 mg/kg soil dw (ECHA) [Kl. Score = 2].

The effective concentration (EC50) of SDES in terrestrial plants (Lactuca sativa) in short term toxicity study of 72 hrs. on the basis of reproduction effect was estimated to be 143.2 mg/kg soil dw (ECHA) [Kl. Score = 2].

Considering that the chemical is readily biodegradable in soil, it is expected that the chemical SDES shall not exhibit toxicity to soil microorganism, terrestrial plants, terrestrial arthropods and soil microorganisms (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium lauryl polyoxyethylene ether sulfate is readily biodegradable; thus, it does not meet the screening criteria for persistence.

No data are available on bioaccumulation. However, based on the low log K_{ow} and calculated BCFs, bioaccumulation is not expected. Thus, sodium lauryl polyoxyethylene ether sulfate does not meet the screening criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on sodium lauryl polyoxyethylene ether sulfate are >0.1 mg/L. The EC_{50} values for sodium lauryl polyoxyethylene ether sulfate are > 1 mg/L. Thus sodium lauryl polyoxyethylene ether sulfate, does not meet the criteria for toxicity.

Therefore, SDS is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium lauryl polyoxyethylene ether sulfate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium lauryl polyoxyethylene ether	9004-82-4	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data from read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (CAS No. 3088-31-1) was used.

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
CFR	Code of Federal Regulations
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mL	grams per millilitre
GLP	good laboratory procedure
GRAS	generally recognized as safe

IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
mbar	millibar
mg/kg dw	milligrams per kilogram dry weight
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SDES	sodium 2-(2-dodecyloxyethoxy) ethyl sulfate
SGG	Synthetic Greenhouse Gases
USFDA	United States Food and Drug Administration

SODIUM LIGNOSULFONATE

This dossier on sodium lignosulfonate presents the most critical studies pertinent to use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium lignosulfonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium lignosulfonate (wood pulp) is the extract of bamboo pulping process, which is made by concentrating, modifying, spraying and drying. Sodium lignosulfonate (CAS 8061-51-6) is light yellow (brown) free flowing powder, and easy to dissolve in water. The chemical property of the product is stable, and the long-term sealed storage cannot be decomposed. Lignin series product is a kind of surfactant, a variety of products can be produced by modification, processing and compounding. These products are mainly used for resin, rubber, dyes, pesticides, ceramics, cement, asphalt, feed, water treatment, water coal slurry, concrete, refractory materials, oil drilling, compound fertilizer, smelting, casting and adhesive. It has been proven by experiment that lignosulfonate is very effective in preventing sandy soil and can be used as a desert fixed sand agent.

As a concrete water-reducing agent sodium lignosulfonate belongs to anionic surface active substance, has adsorption and dispersion effect on cement, and can improve various physical properties of concrete. Sodium lignosulfonate (CAS 8061-51-6) can reduce water consumption by more than 13%, improve the workability of concrete and greatly reduce the hydration heat at the early stage of cement hydration. It can be compounded into early strength agent, retarder, antifreeze, pumping agent, etc. In drilling it can be used as a diluting dispersant and viscosity reducer which can improve petroleum fluidity thereby reducing energy consumption.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium lignosulfonate

CAS RN: 8061-51-6

Molecular formula: Not applicable.

Molecular weight: Unknown

Synonyms: Sodium lignosulfonate; lignosulfonic acid, sodium salt; lignin sodium sulfonate

3 PHYSICO-CHEMICAL PROPERTIES

Sodium lignosulfonate is water soluble (>500 g/L) and has an average molecular weight of 10,000 g/mol (FR, 2005).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium lignosulfonate.

NICNAS has assessed sodium hydroxide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No specific data could be located on the environmental fate/transport of sodium lignosulfonate. The United States Environmental Protection Agency (USEPA) reviewed the environmental fate and environmental hazards of various lignosulfonate chemicals, including sodium lignosulfonate, for a proposed rule to establish 44 tolerance exemptions for residues of these substances (FR, 2005). The USEPA determined “that the various salts of lignosulfonic acid are soluble to very highly water soluble depending on the cation. Once in water, dissociation of the cation is expected depending on pH. These lignosulfonates are not expected to be mobile in terrestrial environments, moving equally with the water and sediment phase to surface water. Ground water migration is not likely. Once in water, the dissociated cation and anion are likely to remain in dissolution. The available information suggest that lignosulfonates may be persistent in aquatic environment of low microbial activity and much less persistent in environments with ample microbial activity…though the time for complete aerobic degradation is predicted to be months, the lignosulfonates are strongly absorbed to soils and sediments due to their high-molecular weights.” Based on the USEPA assessment, it is concluded that sodium lignosulfonate would meet the EU screening criteria for persistence. However, natural mechanisms exist that degrade these polymers and they are considered to be of low risk for the environment.

Due to its high-molecular weight, sodium lignosulfonate is not expected to be bioavailable to environmental receptors. This is supported by pharmacokinetic data on calcium lignosulfonate

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=8061-51-6%2C+

which showed that it is poorly absorbed from the gastrointestinal tract of rats (Beck and Rossi, 2005). Thus, it is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium lignosulfonate is not expected to bioaccumulate due to its low potential for bioavailability because of its molecular weight and size. No aquatic toxicity studies are available for sodium lignosulfonate. It is expected to be a low concern of toxicity to aquatic organisms because of its low potential for bioavailability.

B. Aquatic Toxicity

Limited information is available. SDS is not inherently toxic to algae and invertebrates. It has low toxicity to fish (Golden orfe (*Leuciscud idus*)) with a reported LC_{50} value 1,400 – 2,000 mg/L (Hamburger et al., 1977).

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Based on the assessment by the USEPA (FR, 2005), sodium lignosulfonate meets the criteria for persistence.

Sodium lignosulfonate is not expected to bioaccumulate due to its low potential for bioavailability because of its molecular weight and size. Thus, it does not meet the criteria for bioaccumulation.

Limited aquatic toxicity studies are available for sodium lignosulfonate. It is expected to be a low concern of toxicity to aquatic organisms based on reported LC_{50} values.

The overall conclusion is sodium lignosulfonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium lignosulfonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Lignosulfonate	8061-51-6	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

SODIUM NITRITE

This dossier on sodium nitrite presents the most critical studies pertinent to the risk assessment of sodium nitrite in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium nitrite was assessed as a tier 2 chemical for acute toxicity and as a tier 1 chemical for chronic toxicity. The aquatic toxicity of sodium nitrite is dissipated by dissociation to naturally occurring cations and anions under environmental conditions which further are reduced anaerobically. Therefore, sodium nitrite is classified overall as a **tier 1** chemical based on the preponderance of data and requires a hazard assessment only.

1 BACKGROUND

Sodium nitrite ($NaNO_2$) dissociates completely in aqueous solutions to sodium (Na^{++}) and nitrite (NO_2^{2-}) ions. In the environment, bacteria of the genus Nitrobacter oxidises nitrites to nitrates. Nitrates are reduced to nitrogen by anaerobic bacteria present in soil and sediment. Biodegradation is not applicable to sodium nitrite. Sodium nitrite and its dissociated ions are ubiquitous in the environment. They are not expected to adsorb to soil or sediment and have a low potential for bioaccumulation. Toxicity of sodium nitrite is species and water quality dependant. In particular, chloride ion concentration has been shown to be important, with increasing concentrations leading to a decrease in the toxicity of nitrite.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium nitrite

CAS RN: 7632-00-0

Molecular formula: $NaNO_2$

Molecular weight: 69 g/mol

Synonyms: Sodium nitrite; nitrous acid, sodium salt; nitrous acid sodium salt (1:1)

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Nitrite

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White orthorhombic crystals	2	ECHA

Property	Value	Klimisch score	Reference
Melting Point	271°C @ 101.3 kPa	2	ECHA
Boiling Point	>320°C (decomposes)	2	ECHA
Density	2170 kg/m^3 (temperature not provided)	4	ECHA
Vapour Pressure	9.9 x 10^{-15} Pa @ 25 °C	2	ECHA
Partition coefficient (log K_{ow})	Not applicable	-	ECHA
Water Solubility	848 g/L @ 25°C 820 g/L @ 20°C (pH 9) 666 g/L @ 20°C (pH 9)	2	ECHA
Dissociation Constant (pKa)	Not applicable	'-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium nitrite.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium nitrite is an inorganic salt and will dissociate immediately into sodium and nitrite ions in water. Based on its high water solubility and low vapour pressure, it is unlikely to adsorb to soil or sediment. It has a low potential for bioaccumulation.

B. Partitioning

Sodium nitrite ($NaNO_2$) dissociates completely in aqueous solutions to sodium (Na^{++}) and nitrite (NO_2^{2-}) ions. In the environment, bacteria of the genus *Nitrobacter* oxidises nitrites to nitrates. Nitrates are reduced to nitrogen by anaerobic bacteria present in soil and sediment.

After evaporation or exposure to the air, sodium nitrite will be slowly degraded by photochemical processes (half-life of 82.3 days).However, since sodium nitrite shows a very low vapour pressure evaporation is negligible; therefore, phototransformation in air is of minor importance (ECHA).

C. Biodegradation

Sodium nitrite is an inorganic salt that dissociates completely to sodium and nitrite ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and nitrite ions are also ubiquitous and are present in most water, soil and sediment.

D. Environmental Distribution

Based on the chemical structure and properties an adsorption to soil particles is not expected. Furthermore, sodium nitrite dissociate in the environment immediately into sodium and nitrite ions. Nitrite will be rapidly transformed into nitrate by microbiological activity; thus, adsorption of sodium nitrite is unlikely. Therefore, based on the very high water solubility and the very low vapour pressure sodium nitrite will be mainly distributed in water (ECHA).

E. Bioaccumulation

Sodium nitrite has an estimated BCF of 3.162. Sodium nitrite is known to be metabolised in fish, hence there is low potential for bioaccumulation (OECD SIDS).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The toxicity of sodium nitrite is species and water quality dependant with the preponderance of the data reflecting effective concentrations in the part per million range.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sodium nitrite.

Table 3 Acute Aquatic Toxicity Studies on Sodium Nitrite

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	0.54 – 26.3*	2	ECHA
Channel catfish	96-hour LC_{50}	35	2	ECHA
Tilapia	96-hour LC_{50}	79.8	2	ECHA
Largemouth Bass	96-hour LC_{50}	691	2	ECHA
Daphnia magna	48-hour EC_{50}	15.4	1	ECHA
Cherax quadricarinatus	96-hour LC_{50}	4.93	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50} NOEC	>100 100	1	ECHA

*Four series of 96-hour bioassays were conducted. Series I (12 tests) and Series II (22) tests were conducted over the pH range 6.4 to 9.0. The two series were conducted on two different size ranges of fish and in two different years. Series III (6 tests) was conducted at pH 7 using three different acids (H_2SO_4, H_3PO_4 and HNO_3) for pH reduction. Series IV (4 tests) was conducted over the pH range 7.5 – 8.6 at chloride concentrations above background. Values were converted from NO_2-N to $NaNO_2$.

For sodium nitrite a large number of studies on toxicity to fish are reported in an OECD SIDS dossier. The LC_{50} values obtained vary widely between the species tested. The reason for this difference has been attributed to the ability of certain species, such as eels, bass and sunfish to prevent nitrite from crossing the gill membrane and entering the blood, whilst other species such as rainbow trout concentrate nitrite in their blood. As shown in Table 3, the most sensitive species was the rainbow trout (*Oncorhynchus mykiss*). The wide range of this result is probably depending on the quality of water used in the test system (pH, chloride and calcium ion concentration all having an influence). In particular, chloride ion concentration has been shown to be important, with increasing concentrations leading to a decrease in the toxicity of nitrite. This could also explain why tests with marine species showed a low toxicity to fish compared to some freshwater species (ECHA).

As with fish, there is variation in toxicity between invertebrate species. Sodium nitrite is toxic to invertebrates such as *Cherax quadricarinatus* (LC_{50} (96h) = 4.93 mg NaNO2/L and *Thamnocephalus platyurus* (LC_{50} (24h) = 3.9 mg NaNO2/L), whereas other species, such as *Procambarus clarkii* (LC_{50} (96h) = 18.7 mg NaNO2/L) and *Penaeus paulensis* are much less sensitive (LC_{50} (96h) = 539.2 mg NaNO2/L). Similar to fish, the presence of chloride ions has been found to mitigate nitrite toxicity in some species (OECD SIDS).

Chronic Studies

The 29-day NOEC from a chronic fish study using carp was 21 mg/L as sodium nitrite. The 29-day NOEC from the same study based on physiological changes, especially delayed early ontogeny accompanied by slightly decreased Fulton's condition factor, was 1.05 mg/L as sodium nitrite (Kroupova *et al.*, 2010; ECHA). [Kl. score = 2]

The 31-day NOEC from a chronic fish study using channel catfish was 6.16 mg/L as sodium nitrite based on growth rate (Colt *et al*., 1981; ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium nitrite is an inorganic salt that dissociates completely to sodium and nitrite ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and nitrite ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

As sodium nitrite dissociates to sodium nitrite ions, neither sodium nitrite nor its dissociated ions are expected to accumulate. Based on an estimated BCF value of 3.162, it does not meet the screening criteria for bioaccumulation.

The NOEC values from chronic fish studies on sodium nitrite are >0.1 mg/L. The acute EC_{50} values for sodium nitrite are >1 mg/L in fish, invertebrates and algae. Thus, sodium nitrite does not meet the screening criteria for toxicity.

The overall conclusion is that sodium nitrite is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium nitrite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Nitrite	7632-00-0	Not a PBT	No	No	NA	No	No	No	2	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Colt, R.L., Ludwig, R., Tchobanoglous, G., and Cech, J.J., Jr. (1981). The effects of nitrite on the short-term growth and survival of channel catfish. Aquaculture 24: 111-122.

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Kroupova, H., Machova, J., Packova, V., Blahova, J., Novotny, L., and Svobodova, Z. (2010). Effect of nitrite on early-life stages of common carp (*Cyprinus carpio*). Environ. Toxicol. Chem. 29: 1-6.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

OECD SIDS. SIDS Initial Assessment Report for Sodium Nitrite (CAS No. 7632-00-0). July 2005.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal

LC	lethal concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Cooperation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SID	Screening information dataset
SGG	Synthetic Greenhouse Gases

SODIUM PERSULFATE

This dossier on sodium persulfate presents the most critical studies pertinent to the risk assessment of sodium persulfate in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium persulfate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium persulfate dissociates in aqueous media to the sodium cation (Na+) and persulfate anion ($S_2O_8^{2-}$). The persulfate anion will readily hydrolyse (decompose) into sulfate ions. Biodegradation is not applicable to inorganic compounds. Sodium persulfate is not expected to bioaccumulate; it will dissociate (and decompose) to ions that are ubiquitous in the environment. Sodium persulfate is not expected to absorb to soil or sediment because of its dissociation properties, instability (hydrolysis) and high water solubility. Sodium persulfate exhibits moderate acute toxicity by the oral route and low acute toxicity by the inhalation and dermal routes. In humans, sodium persulfate has the potential for skin irritation; it is also a skin sensitiser to guinea pigs and humans. Human exposure to persulfates (including sodium persulfate) have been linked to a variety of skin and respiratory complaints indicative of sensitisation. The complaints consist of immediate and delayed contact hypersensitivity, contact urticarial, rhinitis, bronchitis and asthma. Repeated oral exposure to sodium persulfate resulted in irritation to the gastrointestinal tract; and respiratory irritation was seen in rats repeatedly exposed by inhalation to ammonium persulfate. Sodium persulfate is not genotoxic. A dermal carcinogenicity study showed no carcinogenic effects in mice. In a screening study, there was no reproductive or developmental toxicity in rats given oral gavage doses of ammonium persulfate. Sodium persulfate has a low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium [(sulfonatoperoxy)sulfonyl]oxidanide

CAS RN: 7775-27-1

Molecular formula: $O_8S_2.2Na$

Molecular weight: 238.1 g/mol

Synonyms: Sodium persulfate; disodium persulfate; sodium peroxodisulfate; disodium [(sulfonatoperoxy)sulfonyl]oxidanide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Persulfate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline, odorless solid	1	ECHA
Melting point	Decomposes at 180°C @ 101.1 kPa before melting point is reached.	1	ECHA
Boiling point	No value determined	-	ECHA
Density	1680 kg/m^3 @ 20 °C	1	ECHA
Vapour pressure	Negligible	2	ECHA
Partition coefficient (log K_{ow})	Not applicable	-	-
Water solubility	730 g/L @ 25 °C (Very soluble)	2	ECHA
Dissociation constant (pKa)	Not applicable	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium persulfate.

NICNAS has assessed sodium persulfate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7775-27-1%2C+

5 ENVIRONMENTAL FATE SUMMARY

Sodium persulfate dissociates in aqueous media to the sodium cation (Na^+) and persulfate anion ($S_2O_8^{2-}$) (OECD 2005; ECHA). The persulfate anion will readily hydrolyse (decompose) into sulfate ions.

The rates of hydrolysis are expected to be similar for sodium persulfate, potassium persulfate, and ammonium persulfate. The rates of decomposition (hydrolysis) were measured at 50°C at various pHs. The half-lives increased from 20 hours at pH 1 to 210 hours at pH 10 (Koltoff and Miller, 1951).

Biodegradation is not applicable to inorganic compounds. Sodium persulfate is not expected to bioaccumulate; it will dissociate (and decompose) to ions that are ubiquitous in the environment. Sodium persulfate is not expected to absorb to soil or sediment because of its dissociation properties, instability (hydrolysis), and high water solubility.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium persulfate has a low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on sodium persulfate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Persulfate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LC_{50}	163	1	ECHA
Daphnia magna	48-hour EC_{50}	133	1	ECHA
Selenastrum capricornutum	72-hour EC_{50}	116	1	ECHA

Chronic Studies

No data are available for sodium persulfate. A 21-day EC_{10} value in Daphnia magna was 25.9 mg/L was reported for diammonium peroxodisulphate (APS) (read-across) (ECHA) [Kl. Score = 1].

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium persulfate is an inorganic compound that dissociates completely to sodium and persulfate ions in aqueous solutions. Persulfate ions are further hydrolysed to sulphate ions. Biodegradation is not applicable to these compounds. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to sodium persulfate or its dissociated compounds.

Sodium persulfate is an inorganic compound that dissociates completely in water to ionic compounds that are ubiquitous in the environment. Thus, sodium persulfate is not expected to bioaccumulate and does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity data on sodium persulfate. Chronic EC_{10} values for invertebrates from a read-across substance (APS) was >0.1 mg/L. The acute EC50 values for fish, invertebrates, and algae are >1 mg/L. Thus, sodium persulfate does not meet the screening criteria for toxicity.

Therefore, sodium persulfate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium persulfate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Persulfate	7775-27-1	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Koltoff, I., and Miller, I.K. (1951). The chemistry of persulfate. I. The kinetics and mechanism of the decomposition of the persulfate ion in aqueous medium. J. Am. Chem. Soc. 73: 3055-3059.

OECD. (2005). IUCLID Data Set for Ammonium persulfate (CAS No. 7727-54-0); Potassium persulfate (CAS No. 7727- 27-1); Sodium persulfate (CAS No. 7775-27-1), UNEP Publications. Available at: https://hpvchemicals.oecd.org/UI/SIDS_Details.aspx?id=5D4B16BE-8BA8-4BE4-8787-469DE31A76E9

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre

PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SODIUM POLYACRYLATE

This dossier on sodium polyacrylate presents the most critical studies pertinent to the risk assessment of sodium polyacrylate in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the HERA document on polyacrylic acid homopolymers and their sodium salts (CAS 9003-04-7) (HERA, 2014). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium polyacrylate is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium polyacrylate are a group of polymers that range in molecular weight from 1,000 to 78,000 g/mol. The sodium polyacrylates mostly used in detergents have a typical molecular weight of approximately 4,500 g/mol (HERA, 2014). These polymers are not readily biodegradable but are partly accessible to ultimate biodegradation. They are not expected to bioaccumulate. Sodium polyacrylate exhibits a low toxicity concern for aquatic organisms, terrestrial invertebrates and plants.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1-Propenoic acid, homopolymer, sodium salt

CAS RN: 9003-04-7

Molecular formula: $(C_3H_4O_2)x$-.x-Na

Molecular weight: Variable

Synonyms: 2-Propenoic acid, homopolymer, sodium salt; polyacrylic acid, sodium salt, sodium polyacrylate; acrylic acid, polymers, sodium salt; poly(acrylic acid), sodium salt; polyacrylate sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Sodium polyacrylates are polymers that range in molecular weight (MW) from 1,000 to 78,000 g/mol (HERA, 2014). The sodium polyacrylates mostly used in detergents have a typical molecular weight of approximately 4,500 g/mol (HERA, 2014). For sodium polyacrylate (MW 4,500), the melting point is >150^{o}C, where it decomposes; and the water solubility is >400 g/L (HERA, 2014).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium polyacrylate.

NICNAS has assessed sodium polyacrylate in an IMAP Tier 1 assessment and considers it a polymer of low concern[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium polyacrylates are not readily biodegradable. Due to their high molecular weights, sodium polyacrylates are not expected to bioaccumulate. In addition, these water-soluble polymers can form insoluble calcium salts in natural waters, suggesting that bioaccumulation is unlikely.

B. Partitioning

Abiotic degradation mechanisms like photolytic and hydrolytic processes do not significantly influence the environmental fate of sodium polyacrylates (HERA, 2014).

C. Biodegradation

Sodium polyacrylates are not readily biodegradable, but are partly accessible to ultimate biodegradation particularly under long incubation conditions. Sodium polyacrylates with MW of <2,000 g/mol are partly biodegradable under the conditions of soil and sediment inoculation. Test results with activated sludge inoculum indicate different elimination degrees, apparently due to adsorption and precipitation processes. The removal degrees of different sodium polyacrylates show no clear relationship between elimination extent and molecular weight (HERA, 2014).

D. Environmental Distribution

Adsorption onto solids and precipitation are the principal mechanisms of abiotic elimination for this type of polymer, the degree of elimination differs and is strongly influenced by test concentration and water hardness (HERA, 2014).

[1] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.

E. Bioaccumulation

No experimental studies are available on sodium polyacrylates. Estimated bioconcentration factors based on octanol-water coefficients are not appropriate since the molecular weights of these polymers are higher than the molecular weight range for the QSAR models. Due to their high molecular weights, sodium polyacrylates are not expected to bioaccumulate. In addition, these water-soluble polymers can form insoluble calcium salts in natural waters, suggesting that bioaccumulation is unlikely (HERA, 2014).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium polyacrylates are a low toxicity concern for aquatic organisms, terrestrial invertebrates and plants.

B. Aquatic Toxicity

Acute Studies

Table 2 lists the results of acute aquatic toxicity studies on sodium polyacrylates.

Table 2 Acute Aquatic Toxicity Studies on Sodium Polyacrylates

Mean MW	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
1,000	*Brachydanio rerio*	96-hour LC_{50}	>200	1	HERA, 2014
1,000	*Salmo gairdneri*	96-hour LC_{50}	>1,000	1	HERA, 2014
1,200	*Leuciscus idus*	96-hour LC_{50}	>500	1	HERA, 2014
2,000	*Brachydanio rerio*	96-hour LC_{50}	>200	1	HERA, 2014
2,500	*Leuciscus idus*	96-hour LC_{50}	>500	1	HERA, 2014
4,500	*Lepomis macrochirus*	96-hour LC_{50}	>1,000	1	HERA, 2014
4,500	*Lepomis macrochirus*	96-hour LC_{50}	>1,000	1	HERA, 2014
8,000	*Leuciscus idus*	96-hour LC_{50}	>500	1	HERA, 2014
10,000	*Lepomis macrochirus*	96-hour LC_{50}	>1,000	1	HERA, 2014
15,000	*Leuciscus idus*	96-hour LC_{50}	>10,000	1	HERA, 2014
78,000	*Brachydanio rerio*	96-hour LC_{50}	>400	2	HERA, 2014
1,000	*Daphnia magna*	48-hour EC_{50}	>200	1	HERA, 2014
1,000	*Daphnia magna*	48-hour EC_{50}	>1,000	1	HERA, 2014
2,000	*Daphnia magna*	48-hour EC_{50}	>200	1	HERA, 2014
4,500	*Daphnia magna*	48-hour EC_{50}	>200	1	HERA, 2014
4,500	*Daphnia magna*	48-hour EC_{50}	>1,000	1	HERA, 2014
78,000	*Daphnia magna*	24-hour EC_{50}	276	2	HERA, 2014
8,000	*Selenastrum*	72-hour EC_{50}	40	1	HERA, 2014

Mean MW	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
	capricornutum				
78,000	*Scenedesmus subspicatus*	96-hour EC_{50}	44	2	HERA, 2014

Chronic Studies

Table 3 lists the results of chronic aquatic toxicity studies on sodium polyacrylates.

Table 3 Chronic Aquatic Toxicity Studies on Sodium Polyacrylates (HERA, 2014)

Mean MW	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
4,500	*Pimephales promelas*	32-day NOEC	56	2	HERA, 2014
4,500	*Brachydanio rerio*	28-day NOEC	>450	1	HERA, 2014
78,000	*Brachydanio rerio*	14-day NOEC	>400	2	HERA, 2014
4,500	*Daphnia magna*	21-day NOEC	450	1	HERA, 2014
4,500	*Daphnia magna*	21-day NOEC	58	1	HERA, 2014
4,500	*Daphnia magna*	21-day NOEC	12	2	HERA, 2014
78,000	*Daphnia magna*	21-day NOEC	100	2	HERA, 2014
4,500	*Scenedesmus subspicatus*	96-hour NOEC	180	2	HERA, 2014
78,000	*Scenedesmus subspicatus*	96-hour NOEC	32.8	2	HERA, 2014

There is considerable variability in the chronic aquatic toxicity results for *Daphnia magna* for sodium polyacrylates with the same molecular weight of 4,500. This was discussed in HERA (2014) and was explained by the solubility of sodium polyacrylates in water. In distilled water, the solubility of sodium polyacrylates with the molecular weight of 4,500 is >400 mg/L; however, under test conditions water solubility will decrease due to the presence of Ca^{++} and Mg^{++} (as measured by water hardness). In a study by BASF (reviewed in HERA, 2014), the water solubility of sodium polyacrylate (MW 4,500) was determined with radiolabelled compounds in a test system with a calcium concentration of 70 mg/L, which corresponds to the mean water hardness to the media used in an OECD TG 202 test. Under these conditions, the water solubility of sodium polyacrylate was 1.3 mg/L after 24 hours. So, one explanation for the variability of the chronic *Daphnia* studies may be due to differences in water hardness.

C. Toxicity to Sediment Organisms

The 96-hour EC_0 to *Chironomus riparius* (larvae) is >4,500 mg/kg sediment dry weight (HERA, 2014).

D. Terrestrial Toxicity

The results of terrestrial toxicity studies on sodium polyacrylate polymers are listed in Table 4.

Table 4 Terrestrial Toxicity Studies on Sodium Polyacrylates (HERA, 2014)

Mean MW	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
4,500	*Eisenia foetida foetida*	14-day EC_0	1,000	1	HERA, 2014
78,000	*Eisenia foetida andrei*	14-day EC_0	1,000	2	HERA, 2014
78,000	*Brassica rapa*	21-day NOEC	1,000	2	HERA, 2014
4,500	Nitrogen transformation*	28-day EC_{10}	>2,500	1	HERA, 2014
4,500	Carbon transformation*	28-day EC_{10}	>2,500	1	HERA, 2014

*Soil organisms

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The sodium polyacrylates are not readily biodegradable; thus they meet the screening criteria for persistence.

The sodium polyacrylates are expected to have high molecular weights and are not expected to be bioavailable. Thus these polymers do not meet the criteria for bioaccumulation.

Chronic NOECs for fish, daphnia and algae are available for sodium polyacrylates, and the NOEC values are >0.1 mg/L. Thus sodium polyacrylates do not meet the screening criteria for toxicity.

The overall conclusion is that sodium polyacrylates are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium polyacrylate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Polyacrylate	9003-04-7	Not a PBT	No	Yes	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

HERA. (2014). Human & Environmental Risk Assessment (HERA) on ingredients of European household cleaning products. Polycarboxylates used in detergents (Part I): Polyacrylic acid homopolymers and their sodium salts (CAS 9003-04-7). (http://www.heraproject.com/files/HERA_P-AA_final_v3_23012014.pdf)

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
GHS	Globally Harmonised System of Classification and Labelling of Chemicals
IUPAC	International Union of Pure and Applied Chemistry
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
MW	molecular weight
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship

REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TG	Test Guideline

SODIUM POLYNAPHTHALENE SULFONATE

This dossier on sodium polynaphthalene sulfonate presents the most critical studies pertinent to the risk assessment of sodium polynaphthalene sulfonate in its use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium polynaphthalene sulfonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium polynaphthalene sulfonate (SPNS) functions as an emulsion stabilizer, surfactant – dispersing agent, and a surfactant – hydrotrope in cosmetic products. It is used as a raw material in the production of admixtures for the construction industry and is one of the basic ingredients for formulation of chemical admixtures for concrete and mortars. It is defined as the sodium salt of the product obtained by the condensation polymerization of 2-naphthalene sulfonic acid and formaldehyde.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Naphthalenesulfonic acid, sodium salt, polymer with formaldehyde

CAS RN: 9008-63-3

Molecular formula: $(C_{10}H_8O_3S.CH_2O.Na)_x$ [This substance is a polymer.]

Molecular weight: Unknown

Synonyms: Sodium polynaphthalene sulfonate; naphthalenesulfonic acid, sodium salt, polymer with formaldehyde; sodium naphthalenesulfonate-formaldehyde copolymer; naphthalenesulfonic acid sodium salt/formaldehyde polymer; formaldehyde/naphthalenesulfonic acid

3 PHYSICO-CHEMICAL PROPERTIES

According to Hampshire Chemical Corp. (1995), SPNS is made by reacting naphthalene with sulfuric acid under conditions of heat and pressure. Formaldehyde and water are then added to produce the acid polymer under the same conditions of heat and pressure. Caustic is added to the acid polymer resulting in the final product (CIR, 2003).

SPNS is tan or amber in powdered form and brown in liquid form. It is completely soluble with a density of 400 – 700 kg/m^3. The substance has a percent (%) volatility of 3 % to 7 % water (CIR, 2003).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium polynaphthalene sulfonate.

NICNAS has assessed 2-naphthalenesulfonic acid, polymer with formaldehyde, sodium salt in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

As a class, the lower molecular weight/bioavailable non-polymeric ammonium, potassium and sodium naphthalenesulfonate formaldehyde condensate surfactants have the following physicochemical profile:

- Non-volatile
- High melting point
- Not lipophilic, but with increasing log K_{ow} with increasing methylation, going from -0.32 for naphthalenesulfonic acids, reaction products with formaldehyde, sodium salts (CAS No. 91078-68-1) to 0.78 for methylnaphthalene sulfonate (no CAS No.)
- Binds tightly to soil
- Oxidative degradation within 8 hours
- Biodegradable with affinity for water and soil compartments (USEPA, 2017)

6 ENVIRONMENTAL EFFECTS SUMMARY

No data are available for this polymeric substance. In lieu of this lack of information, data are taken from the monomeric subunit, sodium naphthalene-2-sulphonate (CAS RN 532-02-5) though it should be noted that toxicity is likely overestimated when read across from the monomer to the polymer.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=36290-04-7

A. Aquatic Toxicity

Acute toxicity of sodium naphthalene-2-sulphonate to freshwater fish and invertebrates was estimated using USEPA's ECOSAR v1.00 predictor. The 96 hr LC_{50} for freshwater fish was calculated to be 105,000 mg/L [KI Score = 2](ECHA) while the 48 hour EC_{50} for the inverebrate Daphnia Magna was estimated to be 49421.05 mg/L [KI Score = 2](ECHA). Based on the QSAR prediction done using the Danish (Q)SAR Database, the 72 hour EC_{50} for the alga, Pseudokirchnerella subcapitata was estimated to be 4767.52 mg/L [KI Score = 2](ECHA). The 100 hr EC_{50} was determined to be 135 mg/L for Daphnia magna [KI Score=2](ECHA).

B. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium polynaphthalene sulfonate is a polymer; it is not expected to be biodegradable. Thus, it meets the criteria for persistence.

Sodium polynaphthalene sulfonate is not expected to bioaccumulate due to its low potential for bioavailability because of its expected molecular weight and size and low water solubility.

No aquatic toxicity studies are available for sodium polynaphthalene sulfonate. The acute E(L)C50 values for read-across substance sodium naphthalene 2-sulphonate are >1 mg/L in fish, invertebrates and algae. Therefore, it does not meet the screening criteria for toxicity.

The overall conclusion is that sodium polynaphthalene sulfonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium polynaphthalene sulfonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Polynaphthalene Sulfonate	9008-63-3	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only based on a read across to the monomeric subunit, sodium naphthalene-2-sulphonate.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

United States Environmental Protection Agency [USEPA]. (2017). Naphthalenesulfonate Formaldehyde Condensates Potassium Salts; Human Health Risk Assessment and Ecological Effects Assessment to Support Proposed Exemption from the Requirement of a Tolerance When Used as an Inert Ingredient in Pesticide Formulations. Office of Pesticide Programs Registration Division. May 10, 2017

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
ECOSAR	Ecological Structure Activity Relationships (ECOSAR v1) Class Program, Risk Assessment Division of the Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency (U.S. EPA/OPPT).
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
QSAR	Quantitative Structure Activity Relationship

SODIUM SILICATE

This dossier on sodium silicate presents the most critical studies pertinent to the risk assessment of sodium silicate in its use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the OECD-SIDS documents on Soluble Silicates, which includes sodium silicate (OECD, 2004); and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Sodium silicate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium silicate is produced by fusing high purity quartz sand (SiO_2) and sodium carbonate or soda (Na_2CO_3) at temperatures of 1,300 to 1,500^{o}C. The product that is formed is an amorphous glass that can be dissolved in water to produce silicate solutions. Various products of sodium silicate are obtained by varying the mixing ratio of quartz and soda. Sodium silicates are therefore characterised primarily by the SiO_2 to Na_2O ratio, or molar ratio (MR). Soluble silicates are generally not distinct stoichiometric chemical substances (with a specific chemical formula and molecular weight), but glasses or aqueous solutions of glasses (OECD, 2004).

Sodium silicate is an amorphous glass, and it is solidified as a glass from the melt (solid or lump glasses). It is essentially anhydrous and differs from ordinary glasses in that it is soluble in water at elevated temperature and pressure leading to silicate solutions (liquid glasses). Both solid and liquid glasses are often referred to as waterglass. Silicate solutions are defined by their density and viscosity, which together with the MR defines a unique composition for the silicate solution. By evaporation of silicate solutions, fine powders or granules are obtained that have a residual water content of approximately 20%. Unlike ground lump glass, these materials dissolve readily in water to give silicate solutions (OECD, 2004).

Upon dissolution in water, sodium silicate forms sodium ions (Na+) and molecular speciation of silicates. Depending on both pH and concentration the respective solutions contain varying proportions of monomeric tetrahydral ions, oligomeric linear or cyclic silicate ions (OECD, 2004).

Sodium silicate has many uses. In concrete and general masonry, it helps to reduce porosity in most masonry products such as concrete, stucco and plasters. Sodium silicate is frequently used in drilling fluids to stabilize borehole walls and to avoid the collapse of bore walls. It is particularly useful when drill holes pass through argillaceous formations containing swelling clay minerals such as smectite or montmorillonite.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium hydroxysilanoylolate

CAS RN: 1344-09-8

Molecular formula: $Na_2O \times nO_2Si$

Molecular weight: 184.04 g/mol (tetrasodium orthosilicate); soluble silicates are not generally stoichiometric chemical substances (with a specific chemical formula and molecular weight), but rather glasses or aqueous solutions of glasses.

Molar ratio: 0.5 for tetrasodium orthosilicate. Commercial sodium silicates have molar ratios between 1.5 and 4.0.

Synonyms: Water glass; soluble glass; silicate of soda; sodium orthosilicate; sodium silicate glass.

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Sodium Silicate

Property	Value	Klimisch score	Reference
Physical state	Amorphous glass melt (lumps); aqueous solution or spray-dried powder with ~20% residual water	4	OECD, 2004
Flow Point	730-870°C	4	OECD, 2004
Melting Point*	Slightly lower than that of water	4	OECD, 2004
Density	1260 – 1710 kg/m^3 (solutions); 700-800 kg/m^3 (bulk density; spray-dried powders) (temperature not provided)	4	OECD, 2004
Vapour Pressure	Negligible at ambient temperature	4	OECD, 2004
Partition Coefficient (log K_{ow})	Not relevant	-	OECD, 2004
Water Solubility	Solution: infinitely miscible; spray-dried solution: readily dissolvable	4	OECD, 2004

*Aqueous solutions

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium silicate.

NICNAS has assessed sodium silicate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=1344-09-8

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium silicate readily dissolves in water to sodium ions (Na^+) and molecular speciation of silicates. Dissolved silica from commercial soluble silicates is indistinguishable from natural dissolved silica. Silica (SiO_2) represents about 59% of the elemental composition of the earth's crust. Similar percentages are obtained for many sediments and soils (Jackson, 1964). Compounds of silicon and oxygen are ubiquitous in the environment; it is present in inorganic matter, like minerals and soils and in organic matter.

Silica is found in all natural waters and the median values in the United States were reported to be 17 mg SiO_2/L for ground waters and 14 mg SiO_2/L for streams (Davis, 1964). The world-wide concentration in rivers is 13 mg SiO_2/L (Edwards and Liss, 1973).

Sodium silicate is an inorganic substance and therefore not amenable to biodegradation. It is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium silicate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sodium silicate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Silicate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Brachydanio rerio	96-hour LC_{50}	1,180	2	OECD, 2004; ECHA
Oncorhynchus mykiss	96-hour LC_{50}	260 - 310	2	ECHA
Daphnia magna	48-hour EC_{50}	1,700	2	OECD, 2004; ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Scenedesmus subspicatus	72-hour EC_{50}	>345.4 (growth rate) 207 (biomass)	2	OECD, 2004; ECHA

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

There are no studies on sodium silicate. A honeybee acute contact toxicity study according to (USEPA, 2012) has been conducted on AgSil™ 25 potassium silicate solution (29.1% potassium silicate in water). The 48-hr LD_0 was 25 µg/animal and the 48-hr LD_{50} was 25 µg/animal (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium silicate is an inorganic compound that dissociates completely to sodium and silicate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and silicate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic compound.

Sodium and silicate ions are essential to all living organisms and are ubiquitous in the environment. Therefore, sodium silicate is not expected to bioaccumulate.

No chronic toxicity data exist on sodium silicate; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Therefore, sodium silicate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium silicate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium silicate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium silicate	1344-09-8	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Davis, S.N. (1964). Silica in streams and ground water. Am. J. Sci. 262: 870-891.

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

Edwards, A.M.C., and Liss, P.S. (1973). Evidence of buffering of dissolved silicon in fresh waters. Nature 243: 341-342.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Jackson, M. L. (1964) Chemical composition of soils. Ch. 2 in Chemistry of the Soil, F. E. Bear, Editor. Rheinhold Publishing Corp., New York, 71–141.Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

OECD. (2004). OECD SIDS Initial Assessment Report (SIAR) and IUCLID Data Set for Soluble Silicates, UNEP Publications.

USEPA. (2012). Ecological Effects Test Guidelines. OCSPP 850.3020: Honey Bee Acute Contact Toxicity Test. January.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilograms per cubic metre

L	litre
LC	lethal concentration
LD	lethal dose
m	metre
mg/L	milligrams per litre
MR	molar ratio
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
USEPA	United States Environmental Protection Agency
µg	micrograms

SODIUM SULFATE

This dossier on sodium sulfate presents the most critical studies pertinent to the risk assessment of sulfate in its use hydraulic fracturing fluids and as a cement additive chemical. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on sodium sulfate (OECD, 2005a,b), and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion: Sodium sulfate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium sulfate dissociates in aqueous media to sodium (Na+) and sulfate (SO_4^{2-}) ions in water. Biodegradation is not applicable to inorganic compounds. Sodium sulfate is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Sodium sulfate is not expected to absorb to soil or sediment because of its dissociation properties and high water solubility. Sodium sulfate is of low acute concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium sulfate

CAS RN: 7757-82-6

Molecular formula: Na_2SO_4

Molecular weight: 142.04 g/mol

Synonyms: Sodium sulfate; disodium sulfate; sodium bisulfate; sulfuric acid, disodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Sulfate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White crystalline solid	2	ECHA
Melting Point	ca. 884°C (pressure not reported)	2	ECHA
Density	2700 kg/m^3 @ 20°C	2	ECHA
Partition Coefficient (Log Kow)	-4.38 (temperature not provided)	2	ECHA
Water Solubility	445.5 g/L @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium sulfate.

NICNAS has assessed sodium sulfate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium sulfate dissociates in aqueous media to sodium (Na^+) and sulfate (SO_4^{2-}) ions. Biodegradation is not applicable to inorganic compounds. Sodium sulfate is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Sodium sulfate is not expected to absorb to soil or sediment because of its dissociation properties and high water solubility.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium sulfate is of low acute concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sodium sulfate.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7757-82-6%2C+

Table 3 Acute Aquatic Toxicity Studies on Sodium Sulfate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	7,960	2	Mount *et al.* (1997)
Daphnia magna	48-hour EC_{50}	4,736*	2	Davies and Hall (2007)

* Standard test conditions: 100 mg $CaCO_3$/L and Ca:Mg ratio of 0.7.

Chronic Studies

The 7-day LOEC from a *Ceriodapnia dubia* reproduction study, in which the test media contained varying degrees of water hardness, was 1,329 mg/L. The NOEC was extrapolated to be approximately 1,109 mg/L (Soucek, 2007).

C. Sediment Toxicity

The lowest 96-hour LC_{50} value to *Hyalella azteca* in a series of studies involving different hardnesses of water was 757 mg/L (Soucek and Kennedy, 2005). In another study with *Hyalella azteca*, the lowest 96-hour LC_{50} value (in water with the lowest hardness) was 841 mg/L (Davies and Hall, 2007). The lowest 96-hour LC_{50} value to *Chironomus tentans* in a series of studies involving different hardnesses of water was 20,899 mg/L (Soucek and Kennedy, 2005).

D. Terrestrial Toxicity

No adequate studies were located.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium sulfate is an organic salt that dissociates completely to sodium and sulfate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both sodium and sulfate ions are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to sodium sulfate or its dissociated ions.

Sodium and sulfate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Thus, sodium sulfate is not expected to bioaccumulate.

The NOEC from a chronic toxicity study with *Ceriodaphnoa rerio* is >0.1 mg/L. The acute EC_{50} values for fish and *Daphnia* are >1 mg/L. Thus, sodium sulfate does not meet the criteria for toxicity.

Therefore, sodium sulfate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium sulfate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium sulfate	7757-82-6	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Davies, T.D., and Hall, K.J. (2007). Importance of calcium in modifying the acute toxicity of sodium sulphate to hyalella Azteca and Daphnia magna. Environ. Toxicol. Chem. 26: 1243-1247.

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Mount, D.R., Gulley, D.D., Hockett, J.R., Garrison, T.D., and Evans, J.M. (1997). Statistical models to predict the toxicity of major ions to Ceriodaphnia dubia, Daphnia magna and Pimephales promelas (Fathead minnows). Environ. Toxicol. Chem. 16: 2009-2019.

OECD. (2005a). Screening Information Dataset (SIDS) Initial Assessment Report for Sodium sulfate (CAS No. 7757-82-6), UNEP Publications.

OECD. (2005b). IUCLID Data Set for Sodium sulfate (CAS No. 7757-82-6), UNEP Publications.

Soucek, D.J. (2007). Comparison of hardness and chloride regulated acute effects of sodium sulfate on two freshwater crustaceans. Environ. Toxicol. Chem. 26: 773-779.

Soucek, D.J., and Kennedy, A.J. (2005). Effects of hardness, chloride, and acclimation on the acute toxicity of sulfate to freshwater invertebrates. Environ. Toxicol. Chem. 24: 1204-1210.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts

EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
LOEC	lowest observed effective concentration
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set

SODIUM SULPHITE

This dossier on sodium sulphite presents the most critical studies pertinent to the risk assessment of sodium sulphite in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium sulphite is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium sulphite readily dissociates in aqueous media to the sodium (Na+) and sulphite (SO_3^{2-}) ions. At neutral pH, a mixture of 50% sulphite (SO_3^{2-}) and 50% bisulphite (HSO_3^{2-}) is present. In surface waters, sulphite is oxidized to sulfate either catalytically by air oxygen or by microbial action. The presence of cations like iron, copper or manganese in the environment accelerates the oxidation rate significantly.

Biodegradation is not applicable to inorganic compounds. Bioaccumulation is not to be expected because of the resulting strong anionic nature of the substance, as well as its rapid oxidative transformation to sulfates under physiological and environmental circumstances. Sodium sulphite is of low toxicity concern to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium sulfate

CAS RN: 7757-83-7

Molecular formula: Na_2SO_3

Molecular weight: 126.0 4 g/mol

Synonyms: Sodium sulphite; disodium sulphite; anhydrous sodium sulfite

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Sodium Sulphite

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	2	ECHA
Melting Point	911°C (pressure not provided)	2	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	No data	-	-
Density	2630 kg/m^3 @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	307 g/L @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium sulphite.

NICNAS has assessed sodium sulphite in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium sulphite readily dissociates in aqueous media to the sodium (Na+) and sulphite (SO_3^{2-}) ions. Biodegradation is not applicable to inorganic compounds. Bioaccumulation is not to be expected because of the resulting strong anionic nature of the substance, as well as its rapid oxidative transformation to sulfates under physiological and environmental circumstances. Because of the anionic nature, any quantitatively relevant adsorption onto soil, sediments or suspended matter for sodium sulfite as well as its dissociation products is not to be expected. (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium sulphite is of low toxicity concern to aquatic life.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7757-83-7%2C+

A. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on sodium sulphite.

Table 3: Acute Aquatic Toxicity Studies on Sodium Sulphite and Sodium Disulphite

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Golden orfe	96-hr LC_{50}	316	2	ECHA
Daphnia magna	48-hr EC_{50}	89* (59)	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50}	43.8* (29)	2	ECHA

*Test substance: sodium disulphite

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies conducted on sodium sulphite and sodium disulphite.

Table 4: Chronic Aquatic Toxicity Studies on Sodium Sulphite and Sodium Disulphite

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Zebrafish	34-d NOEC	>316	1	ECHA
Daphnia magna	21-d NOEC	>10* (6.6)	1	ECHA
Desmodesmus subspicatus	EC_{10}	33.3* (22)	2	ECHA

*Test substance: sodium disulphite; adjusted concentration for sodium sulphite in parentheses.

B. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium sulphite dissociates completely to sodium and sulphite ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistence criteria is not considered applicable.

Bioaccumulation is not to be expected because of the resulting strong anionic nature of the substance, as well as its rapid oxidative transformation to sulfates under physiological and

environmental circumstances. Thus, sodium sulphite does not meet the screening criteria for bioaccumulation.

The NOEC or EC_{10} values from chronic aquatic toxicity studies on sodium sulphite is >0.1 mg/L. Thus, sodium sulphite does not meet the criteria for toxicity.

The overall conclusion is that sodium sulphite is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium sulphite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium sulphite	7757-83-7	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.euroa.eu/information-on-chemicals/registered-substances.

European Chemicals Agency (ECHA). (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol, Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

SODIUM THIOSULPHATE

This dossier on sodium thiosulphate presents the most critical studies pertinent to the risk assessment of sodium thiosulphate in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium thiosulphate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium thiosulphate dissociates in aqueous media to sodium (Na^+) and thiosulphate ($S_2O_3^{2-}$) ions. These ionic species are ubiquitous in the environment and are present in most water, soil and sediment mediums. Neither sodium thiosulphate nor its dissociated ions are expected to bioaccumulate. Sodium thiosulphate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Disodium sulphanidesulphonate

CAS RN: 7772-98-7

Molecular formula: $Na_2S_2O_3$

Molecular weight: 158.1 g/mol

Synonyms: Sodium thiosulphate; disodium sulphanidesulphonate; sodium thiosulphate; thiosulphuric acid, disodium salt; disodium sulphurothioate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Thiosulphate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless crystalline solid	2	ECHA
Melting Point	<500°C (decomposition occurs) (pressure not indicated)	1	ECHA
Density	1690 kg/m^3 @ 20 °C	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	764 g/L @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium thiosulphate.

NICNAS has assessed sodium thiosulphate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment. It is an inorganic substance comprising ions of low ecotoxicological concern. This chemical is not expected to pose an unreasonable risk to the environment provided that ANZECC water quality guidelines for physical and chemical stressors are not exceeded.[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium thiosulphate dissociates in aqueous media to sodium (Na^+) and thiosulphate ($S_2O_3^{2-}$) ions. The thiosulphate anion is stable in neutral or alkaline media, but not in acidic media (EPA, 2007). In aqueous media, thiosulphate irreversibly disproportionates to sulphide and sulphate (EPA, 2007).

Biodegradation is not applicable to inorganic compounds. Sodium thiosulphate is not expected to bioaccumulate; it will dissociate to ions that are ubiquitous in the environment. Sodium thiosulphate is not expected to absorb to soil or sediment because of its dissociation properties and high water solubility.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium thiosulphate is of low toxicity concern to aquatic organisms.

[1]https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=7772-98-7

B. Aquatic Toxicity

Acute Studies

No acute studies were identified for sodium thiosulphate. **Table 3** lists the results of acute aquatic toxicity studies conducted on ammonium thiosulphate (CAS No. 7783-18-8).

Table 3: Acute Aquatic Toxicity Studies on Ammonium Thiosulphate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Lepomis macrochirus	96-hr LC_{50}	510	1	ECHA
Salmo gairdneri	96-hr LC_{50}	770	1	ECHA
Daphnia magna	48-hr EC_{50}	230	1	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	>100	1	ECHA

Chronic Studies

No studies were identified for sodium thiosulphate or ammonium thiosulphate. However, reliable chronic toxicity data were available for sodium sulphite (CAS No. 7757-83-7) and sodium disulphite (CAS No. 7757-74-6). Table 4 lists the results of chronic aquatic toxicity studies conducted on sodium sulphite and sodium disulphite.

Table 4: Chronic Aquatic Toxicity Studies on Sodium Sulphite and Sodium Disulphite

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Zebrafish	34-d NOEC	>316	1	ECHA
Daphnia magna	21-d NOEC	>10* (6.6)	1	ECHA
Desmodesmus subspicatus	EC_{10}	33.3* (22)	2	ECHA

*Test substance: sodium disulphite; adjusted concentration for sodium sulphite in parentheses.

C. Terrestrial Toxicity

No studies were identified.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium thiosulphate is an inorganic salt that dissociates completely to sodium, sulphide, and sulphate ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; these ionic species are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistence criteria is not considered applicable.

Sodium thiosulphate dissociates to ionic species. The sulphide ion can be oxidized by bacteria to sulphate. The sodium and sulphate ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Thus, sodium thiosulphate is not expected to bioaccumulate.

The NOEC or EC_{10} values from chronic aquatic toxicity studies on read-across sodium sulphite is >0.1 mg/L. The acute EC(L)50 values on read-across ammonium thiosulphate are >1 mg/L in fish, invertebrates and algae. Thus, sodium thiosulphate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium thiosulphate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium thiosulphate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Thiosulphate	7772-98-7	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).
3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

U.S. EPA [EPA] (2007). Reregistration Eligibility Decision (RED) for Ammonium Thiosulphate, Office of Prevention, Pesticides and Toxic Substances, EPA 738-R-07-001, December 20, 2007.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
mg/L	milligrams per litre
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

BENZENESULFONIC ACID, DIMETHYL-, SODIUM SALT
[SODIUM XYLENE SULFONATE]

This dossier on benzenesulfonic acid, dimethyl-, sodium salt (sodium xylene sulfonate) presents the most critical studies pertinent to the risk assessment of sodium xylene sulfonate in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on Hydrotropes (which includes sodium xylene sulfonate) (OECD, 2005), and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium xylene sulfonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium xylene sulfonate is a UVCB substance that is readily biodegradable and does not bioaccumulate. It is expected to have low potential to bind to sediment and soil. Sodium xylene sulfonate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium 3,4-dimethylbenzenesulfonate

CAS RN: 1300-72-7

Molecular formula: $C_8H_{10}O_3S.Na$

Molecular weight: 208.21 g/mol

Synonyms: Sodium xylene sulfonate; sodium 3,4-dimethylbenzenesulfonate; 3,4-xylenesulfonic acid, sodium salt; sodium dimethylbenzenesulfonate; benzenesulfonic acid, dimethyl; sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Xylene Sulfonate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	1	ECHA
Melting Point	>300°C @ 101.3 kPa	1	ECHA
Boiling Point	-	-	-
Density	984 kg/m^3 @ 20 °C	1	ECHA
Vapour Pressure	Negligible	2	USEPA, 2017

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-3.12 (measured) @ 20 °C	1	ECHA
Water Solubility	664 g/L @ 20°C (pH approximately 11.96)	1	ECHA
Dissociation constant (pKa)	7.1 @ 20°C	1	ECHA

Sodium xylene sulfonate is known as a hydrotrope. Hydrotropes are substances that are amphiphilic, in that they are composed of both a hydrophilic and a hydrophobic functional group. The hydrophobic part of the molecule is a benzene substituted non-polar segment. The hydrophilic polar segment is an anionic sulfonate group that is comparatively a short side chain, accompanied by a counter ion. Hydrotropes are used as coupling agents to solubilise the water-insoluble and often incompatible functional ingredients of household and institutional cleaning products and personal care products. The hydrotropes are not surfactants, but are used to solubilise complex formulas in water (OECD, 2005).

Sodium xylene sulfonate is expected to dissociate completely in aqueous media.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium xylene sulfonate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sodium xylene sulfonate is readily biodegradable and it does not bioaccumulate. It is expected to have low potential to bind to sediment and soil.

B. Partitioning

Hydrotropes are not volatile substances and not subject to hydrolysis. Sodium xylene sulfonate is expected to dissociate completely in aqueous media.

C. Biodegradation

Sodium xylene sulfonate is readily biodegradable. In two separate OECD 301B tests, degradation was 74% in 15 days; and 88% and 84% in 28 days. In the second test, the 60% threshold was attained after 6 days (OECD, 2005; ECHA). [Kl. score = 1]

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for sodium xylene sulfonate. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value of 2,4-dimethylsulfonate and 3,4-dimethylsulfonate from the molecular connectivity index (MCI) and log K_{ow} are 26.3 and 0.7876 L/kg, respectively. Thus, the potential for adsorption to soil or sediment is low. Based on these values along with the sodium xylene sulfonate's high water solubility, if released to water, it will likely preferentially partition into the water column and not adsorb to suspended solids or sediments.

E. Bioaccumulation

No experimental studies have been conducted on sodium xylene sulfonate. Fish bioconcentration tests (OECD TG 305C) have been conducted on similar substances: sodium xylene sulfonate (CAS No. 827-21-4) and sodium toluene sulfonate (CAS No. 12068-03-0). All measured values were lower than the detection limit of the HPLC analysis. The measured BCF values in *Cyprinus* species were <2.3 (OECD, 2005). Thus the substance does not appreciably bioconcentrate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium xylene sulfonate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on sodium xylene sulfonate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Xylene Sulfonate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Rainbow trout	96-hour LC_{50}	>408 a.i.*	2	OECD, 2005
Fathead minnow	96-hour LC_{50}	>400 a.i.	2	OECD, 2005
Daphnia magna	48-hour EC_{50}	>408 a.i.	2	OECD, 2005

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Daphnia magna	48-hour EC_{50}	>400 a.i.	2	OECD, 2005
Selenastrum capricornutum	96-hour EC_{50} NOEC	230 31	2	OECD, 2005

*= active ingredient

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium xylene sulfonate is readily biodegradable; thus it does not meet the screening criteria for persistence.

The BCF values from two separate fish bioconcentrations on similar substances to sodium xylene sulfonate were <2.3. Thus, sodium xylene sulfonate does not meet the criteria for bioaccumulation.

The NOEC from an algal study on sodium xylene sulfonate is >0.1 mg/L. The acute $E(L)C_{50}$ values for sodium xylene sulfonate are >1 mg/L for fish, invertebrates and algae. Thus, sodium xylene sulfonate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium xylene sulfonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium xylene sulfonate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Xylene Sulfonate	1300-72-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

OECD. (2005). SIDS Initial Assessment Report for the Hydrotropes (CAS No. 1300-72-7, 12068-03-0, 26447-10-9m 28348-53-0, 32073-22-6, 37475-88-0) and SIDS Dossier on Xylene sulfonic acid, sodium salt (CAS No. 1300-72-7), UNEP Publications.

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
a.i.	active ingredient
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union

g/L	grams per litre
HPLC	High performance liquid chromatography
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	screening information data set
TG	test guideline

SOYBEAN OIL

This dossier on soybean oil presents the most critical studies pertinent to the risk assessment of soybean oil in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Soybean oil is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Soybean oil is a vegetable oil extracted from the seeds of the soybean (*Glycine max*). Soybean oil is essentially triacylglycerols: fatty acids esterified to glycerol. The major unsaturated and saturated fatty acids in soybean oil are approximately: 56% linoleic acid ($C_{18:2}$), 21% oleic acid ($C_{18:1}$), 10% palmitic acid ($C_{16:0}$), 7% linolenic acid ($C_{18:3}$) and 4% stearic acid ($C_{18:0}$) (Zambiazi et al., 2007).

Manufacturers of both industrial and consumer products use soybean oil to replace petroleum and other volatile or hazardous ingredients, and increase product performance. Soybean oil is used in a variety of applications including rubber, fiber, coatings, solvents, plastics, lubricants and adhesives.

Soybean oil is a substance primarily composed of glycerides. They are expected to be rapidly and ultimately degradable and to have low aquatic toxicity. This substance and its degradation products are unlikely to cause harm in the environment.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Soybean Oil

CAS RN: 8001-22-7

Molecular formula: Not applicable

Molecular weight: Not applicable

Synonyms: A6OIL;CAP 18;D04962;HY 3050;CT 7000;Soy oil; soybean; SOYA OIL; Bionatrol; CLINOLEIC.

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Soybean Oil

Property	Value	Klimisch score	Reference
Physical State	Oily; Colourless to Yellow liquid	2	Chemical Book
Density	917 kg/m^3 @ 25°C (lit.)	2	Chemical Book
Water Solubility	Immiscible with water	2	Chemical Book

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for soybean oil.

NICNAS has assessed soybean oil in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment. Soybean oil is a substance primarily composed of glycerides. They are expected to be rapidly and ultimately degradable and to have low aquatic toxicity. This substance and its degradation products are unlikely to cause harm in the environment[1]

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Environmental fate data was not available for soybean oil. Environmental fate properties were evaluated using read-across for a similar substance in the group: fatty acids, soybean oil, conjugated. Substances in this group similar in chain length to fatty acids found in soybean oil are insoluble,

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments-keywords?keywords=soybean+oil

immobile and have high adsorption to soil and sediment. Fatty acids occur naturally in all aquatic organisms and are ubiquitous in the aquatic environment, where fatty acids are predominantly readily biodegraded in an aerobic environment by microorganisms. As fatty acids are naturally stored in the form of triacylglycerols primarily within fat tissue until they are used for energy production (fat storage tactic), it is therefore considered that there will be no risk to aquatic organisms from potential bioconcentration/biomagnification of fatty acids (ECHA).

B. Partitioning

In water fatty acids are abiotically stable. Based on high insolubility and molecular structure (aliphatic, mostly saturated carbon chains) hydrolysis is not a relevant degradation pathway. Direct photolysis is not expected to contribute appreciably to the overall breakdown rate in water and soil, since the environmental degradation of these substances is predominantly of biotic nature (ECHA).

C. Biodegradation

The biodegradation data for the members of the fatty acids category includes standard biodegradation studies as well as modelling data (QSAR). The vast majority of the experimental results revealed ready biodegradability which was supported by reliable QSAR predictions. As summarized in the category justification, the members of the fatty acids will predominantly ready biodegrade (ECHA).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

Based on the chemical structure and physical properties (insoluble), soybean oil is expected to have high adsorption to soil or sediment and be immobile. Estimated Koc values for linoleic acid (CAS No. 60-33-3) was 11,360 (ECHA) [Kl. Score = 2].

E. Bioaccumulation

A fish bioaccumulation study is available for the analogue substance C12 fatty acid-sodium laurate which showed negligible evidence of bioaccumulation potential in fish tissues with an estimated BCF of 255 L/kg after 28 days exposure (ECHA) [Kl. Score = 2].

As fatty acids are naturally stored in the form of triacylglycerols primarily within fat tissue until they are used for energy production (fat storage tactic), it is therefore considered that there will be no risk to aquatic organisms from potential bioconcentration/biomagnification of fatty acids (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Soybean oil is expected to readily biodegrade be of low toxicity to environmental receptors.

B. Aquatic Toxicity

No study is available on the aquatic toxicity of fatty acids, soybean oil, conjugated (CAS 1176286 -43 -3) with fish, invertebrates or algae.

Soybean oil is of low acute toxicity concern to fish and invertebrates based on studies conducted on the surrogate compound glycerol trioleate (CAS No. 122-32-7) . The LC_{50} value of glycerol trioleate to fish has been reported to be 10,000 mg/L; and the EL_{50} of glycerol trioleate (WAF) to Daphnia indicates that is considerably greater than its water solubility (Willing et al., 2001).

C. Terrestrial Toxicity

Fatty acids occur in soils naturally, are part of physiological pathways and can be used as energy source. Thus, low toxicity is expected for terrestrial organisms exposed to the test substance (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Soybean oil is expected to degrade in the environment and thus does not meet the criterion for persistence.

There are no specific data on the bioaccumulation potential for soybean oil but its expected degradation and read-across from a similar substance suggests that bioaccumulation is unlikely. Therefore, soybean oil does not meet the criterion for bioaccumulation.

Soybean oil is of low concern for toxicity and does not meet the criterion for this parameter.

The overall conclusion is that soybean oil is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for soybean oil.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Soybean Oil	8001-22-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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Zambiazi, R.C., Przybylski, R., Zambiazi, M.W., and Mendonça, C.B. (2007). Fatty acid composition of vegetable oils and fats. B.CEPPA, Curitiba 25(1): 111-120.

B. Abbreviations and Acronyms

°C	degrees Celsius
°F	degrees Fahrenheit
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre

PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

SOYBEAN OIL, METHYL ESTER, SULFATED, SODIUM SALT

This dossier on soybean oil, methyl ester, sulfated, sodium salt presents the most critical studies pertinent to the risk assessment of this substance in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Soybean oil, methyl ester, sulfated, sodium salt is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Soybean oil, methyl ester, sulfated, sodium salt is derived from soybean oil. Soybean oil is a vegetable oil extracted from the seeds of the soybean (*Glycine max*). Soybean oil is essentially triacylglycerols: fatty acids esterified to glycerol. The major unsaturated and saturated fatty acids in soybean oil are approximately: 56% linoleic acid ($C_{18:2}$), 21% oleic acid ($C_{18:1}$), 10% palmitic acid ($C_{16:0}$), 7% linolenic acid ($C_{18:3}$) and 4% stearic acid ($C_{18:0}$) (Zambiazi et al., 2007).

Limited environmental fate data was available for soybean oil, methyl ester, sulfated, sodium salt. As a result, environmental fate properties were supplemented using read across for a similar substance: fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3). Substances in this group similar in chain length to fatty acids found in soybean oil are insoluble, immobile and have high adsorption to soil and sediment. Fatty acids occur naturally in all aquatic organisms and are ubiquitous in the aquatic environment, where fatty acids are predominantly readily biodegraded in an aerobic environment by microorganisms. As fatty acids are naturally stored in the form of triacylglycerols primarily within fat tissue until they are used for energy production (fat storage tactic), it is therefore considered that there will be no risk to aquatic organisms from potential bioconcentration/biomagnification of fatty acids (ECHA). Low toxicity is therefore expected for aquatic or terrestrial organisms exposed to soybean oil, methyl ester, sulfated, sodium salt.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Soybean oil, methyl ester, sulfated, sodium salt

CAS RN: 68918-47-8

Molecular formula: Not applicable as substance is a UVCB

Molecular weight: Not applicable as substance is a UVCB

Synonyms: Soybean oil, Me ester, sulfated, sodium salt

3 PHYSICO-CHEMICAL PROPERTIES

There are no physical or chemical data for soybean oil, methyl ester, sulfated, sodium salt. Key physical and chemical properties for read-across substance fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3) are provided in Table 1.

Table 1 Overview of the Physico-chemical Properties of Soybean oil, methyl ester, sulfated, sodium salt*

Property	Value	Klimisch score	Reference
Physical State	Yellow, viscous liquid	2	ECHA
Melting Point	6.29°C @ 101.3 kPa	1	ECHA
Boiling Point	354.3°C @ 101.3 kPa	1	ECHA
Density	888 kg/m^3@ 20 °C	1	ECHA
Vapor Pressure	6.8 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	6.2 @ 25°C	1	ECHA
Water Solubility	0.000023 g/L @ 25°C	1	ECHA
Dissociation constant (pKa)	Not Applicable	-	ECHA
Viscosity	6.1 mPa s @ 20°C	2	ECHA

*Based on read-across substance fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3)

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory) under alternate CAS No. 68918-44-5[1]. No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for soybean oil, methyl ester, sulfated, sodium salt.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] Soybean oil, mixed with soybean oil Me esters, sulfated, sodium salts. Also referred to as soybean oil, soybean oil methyl esters, sulfated, sodium salt

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Limited environmental fate data was available for soybean oil, methyl ester, sulfated, sodium salt. As a result, environmental fate properties were supplemented using read across for a similar substance: fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3). Substances in this group similar in chain length to fatty acids found in soybean oil are insoluble, immobile and have high adsorption to soil and sediment. Fatty acids occur naturally in all aquatic organisms and are ubiquitous in the aquatic environment, where fatty acids are predominantly readily biodegraded in an aerobic environment by microorganisms. As fatty acids are naturally stored in the form of triacylglycerols primarily within fat tissue until they are used for energy production (fat storage tactic), it is therefore considered that there will be no risk to aquatic organisms from potential bioconcentration/biomagnification of fatty acids (ECHA).

B. Biodegradation

All methyl esters of fatty acids are readily biodegradable in water, soil and sediments. They pass the 10 days windows with 62% of degradation. Half-life in the three compartment is less than 2 -3 days. In some case even less than 1 day (ECHA). This corresponds with chemical-specific data provided for soybean oil, methyl ester, sulfated, sodium salt which indicated that the chemical is readily biodegradable. There was 61% degradation after 28 days (Halliburton, 2020).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for soybean oil, methyl ester, sulfated, sodium salt. Based on the chemical structure and physical properties (insoluble), soybean oil, methyl ester, sulfated, sodium salt is expected to have high adsorption to soil or sediment and be immobile. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated log K_{oc} value from the molecular connectivity index (MCI) and log K_{ow} methods[2] are 12.8 and 10.5 L/kg, respectively, for similar substance soybean oil, mixed with soybean oil Me esters, sulfated, sodium salts (CAS No. 68918-44-5).

D. Bioaccumulation

A fish bioaccumulation study is available for read-across substance fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3) which showed low bioaccumulation potential in fish tissues with an estimated BCF of 3 L/kg after 20 days exposure (ECHA) [Kl. Score = 2].

Fatty acids are naturally stored in the form of triacylglycerols primarily within fat tissue until they are used for energy production (fat storage tactic), it is therefore considered that there will be no risk to aquatic organisms from potential bioconcentration/biomagnification of fatty acids (ECHA).

[2] Due to the fact that this substance is a long-chain hydrocarbon which exceeds the applicability domain of KOWWIN, the value for log K_{ow} is reported with restrictions.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Low toxicity is expected for aquatic or terrestrial organisms exposed to soybean oil, methyl ester, sulfated, sodium salt.

B. Aquatic Toxicity

Acute Studies

There are no acute studies available on the aquatic toxicity of soybean oil, methyl ester, sulfated, sodium salt with fish, invertebrates, or algae. Table 3 lists the results of acute aquatic toxicity studies conducted on read-across substance fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3).

Table 3 Acute Aquatic Toxicity Studies on Fatty acids, C16-18 and C18-unsaturated, methyl esters (CAS No. 67762-38-3)[a]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	48-hr LC_{50}	100,000 (WAF)	2	ECHA
Daphnia magna	48-hr EC_{50}	2,504 (WAF)	2	ECHA
Raphidocelis subcapitata (previous names: *Pseudokirchneriella subcapitata, Selenastrum capricornutum*)	72-hr EC_{50}	73, 729 (growth rate)	2	ECHA

a – Based on fatty acid read-across substance fatty acids rape oil, methyl ester (CAS number not provided)
WAF – water accommodated fraction

Chronic Studies

No studies are available. Chronic tests were not conducted because of low water solubility, toxicity only for very high concentrations (100,000 mg/L), and the degradation rate (DT_{50} of 5-7 days in freshwater) of the test substance in environmental conditions (ECHA).

C. Terrestrial Toxicity

No studies are available. Fatty acids occur in soils naturally, are part of physiological pathways and can be used as energy source. Thus, low toxicity is expected for terrestrial organisms exposed to the test substance (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Soybean oil, methyl ester, sulfated, sodium salt is expected to be readily biodegradable; thus it does not meet the screening criteria for persistence.

There are no specific data on the bioaccumulation potential for soybean oil, methyl ester, sulfated, sodium salt but its expected degradation and read-across from a similar substance suggests that bioaccumulation is unlikely. Therefore, soybean oil, methyl ester, sulfated, sodium salt does not meet the screening criteria for bioaccumulation.

There are no acute or chronic aquatic toxicity studies on soybean oil, methyl ester, sulfated, sodium salt. However, the acute E(L)C_{50} values are >1 mg/L in similar read-across substances. Thus, the substance does not meet the screening criteria for toxicity.

The overall conclusion is that soybean oil, methyl ester, sulfated, sodium salt is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for soybean oil, methyl ester, sulfated, sodium salt.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Soybean oil, methyl ester, sulfated, sodium salt	68918-47-8	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency

EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L	litre
LC	lethal concentration
mg/L	milligrams per litre
mPa s	millipascal – second
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	unknown or variable composition, complex reaction products or of biological materials

STARCH

This dossier on starch presents the most critical studies pertinent to the risk assessment of starch in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion: Starch is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Starch is a polysaccharide comprised of glucose; it is synthesized in plants during photosynthesis. Starch is expected to be biodegradable and not bioaccumulate. Starch is not toxic to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxyoxane-3,4,5-triol

CAS RN: 9005-25-8

Molecular formula: $(C_6H_{10}O_5)_n$

Molecular weight: Variable, UVCB

Synonyms: Starch, soluble; maltose; corn starch;rice starch; sorghum gum; starch gum' tapioca starch

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Starch (Maltose)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Fine, white odorless powder		PubChem
Melting Point	240°C (pressures not provided)		PubChem
Boiling Point	Decomposes		PubChem
Density	1500 kg/m^3 (temperature not provided)		PubChem
Vapour Pressure	Negligible		PubChem
Water Solubility	Insoluble		PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for starch.

NICNAS has assessed soybean oil in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment.[1]

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Starch is a polysaccharide comprising glucose monomers joined in α-1,4 linkages. The simplest form of starch is the linear polymer amylose; amylopectin is the branched form. Starch is manufactured in the green leaves of plants from excess glucose produced during photosynthesis and serves the plant as a reserve food supply.

When required, starch is broken down, in the presence of certain enzymes and water, into its constituent monomer glucose units, which diffuse from the cell to nourish the plant tissues. In humans and other animals, starch is broken down into its constituent sugar molecules, which then supply energy to the tissues[2].

Starch, which is insoluble in water, is expected to be biodegradable and not bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Starch is non-toxic to aquatic organisms.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9005-25-8
[2] https://www.britannica.com/science/starch

B. Aquatic Toxicity

Acute Studies

Table 2 lists the results of acute aquatic toxicity studies on starch.

Table 2 Acute Aquatic Toxicity studies on Starch

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Orthopristis chrysoptera (pinfish)	96-hour LC_{50}	>5,000 (no mortality)	4	USEPA
Bairdiella chrysoura (silver perch)	96-hour LC_{50}	>5,000 (no mortality)	4	USEPA
Lagodon rhomboids (pinfish)	96-hour LC_{50}	>5,000 (no mortality)	4	USEPA

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Starch is expected to be readily biodegradable. Therefore, it does not meet the screening criteria for persistence.

Starch is a polysaccharide with a high molecular weight (approximately 21,000 to 500,000) daltons which limits its bioavailability to aquatic organisms. Therefore, it is not expected to bioaccumulate.

There are no chronic toxicity studies on starch. The acute LC_{50} values for starch are >1 mg/L. Therefore, starch does not meet the screening criteria for toxicity.

Therefore, starch is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for starch.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Starch	9005-25-8	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts (DEWHA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
LC	lethal concentration
mg/L	milligrams per litre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

Starch, Carboxymethyl Ether

This dossier presents the most critical studies pertinent to the risk assessment of starch, carboxymethyl ether as it relates to its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all the available data. As there are no available studies for starch, carboxymethyl ether, this dossier is based on information obtained from similar read-across substance starch (CAS No. 9005-25-8). Where possible, the study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion- Starch, carboxymethyl ether is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Starch is a polysaccharide comprised of glucose; it is synthesized in plants during photosynthesis. Starch, carboxymethyl ether is a starch derivative in which the -OH groups of the starch molecule are partially substituted by ether group (-O-CH_2COOH).

Starch and starch, carboxymethyl ether are reported to have uses in drilling fluid formulations for fluid loss control and as a gelling agent during fracturing or fracturing pre-treatment.

Starch, carboxymethyl ether is expected to be biodegradable and not bioaccumulate. Starch, carboxymethyl ether is not toxic to aquatic organisms.

2 CHEMICAL AND IDENTIFICATION

Chemical Name (IUPAC): Starch, carboxymethyl ether

CAS RN: 9057-06-1

Molecular formula: $(C_2H_4O_3)_x$

Molecular weight: Variable, UVCB

Synonyms: Carboxymethyl starch; carboxymethylated starch; starch glycolate

3 PHYSICO-CHEMICAL PROPERTIES

Starch is insoluble (ICSC). Chemical modification of starch by carboxymethylation (starch, carboxymethyl ether) increases the inherent chemical properties of starch, such as solubility and thermal stability. Starch, carboxymethyl ether exhibits varying degrees of viscosity depending on its degree of substitution (Spychaj, et al., 2012).

The number average molecular weight (NAMW) of starch, carboxymethyl ether is reported to be greater than 1,000,000 daltons (Adeyanju et al., 2016). No other chemical-specific information is available.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances-ACIS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for starch, carboxymethyl ether.

NICNAS has assessed starch, carboxymethyl ether in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment.[1]

Table 1 Existing International Controls

Convention, Protocol, or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE PROPERTIES

Starch, carboxymethyl ether is a starch derivative in which the -OH groups of the starch molecule are partially substituted by ether group (-O-CH_2COOH). No environmental fate properties are available for starch, carboxymethyl ether. Information for read-across substance starch (CAS No. 9005-25-8) is provided.

Starch is a polysaccharide comprising glucose monomers joined in α-1,4 linkages. The simplest form of starch is the linear polymer amylose; amylopectin is the branched form. Starch is manufactured in the green leaves of plants from excess glucose produced during photosynthesis and serves the plant as a reserve food supply.

When required, starch is broken down, in the presence of certain enzymes and water, into its constituent monomer glucose units, which diffuse from the cell to nourish the plant tissues. In humans and other animals, starch is broken down into its constituent sugar molecules, which then supply energy to the tissues[2].

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=9057-06-1
[2] https://www.britannica.com/science/starch

Starch is expected to be biodegradable. Assuming a molecular weight greater than 1,000 daltons, starch (and starch derivatives) will be unable to cross cell membranes; and, as a result, are unlikely to bioaccumulate (Boethling and Nabholz, 1997).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Starch, carboxymethyl ether exhibits low toxicity to aquatic organisms.

B. Aquatic Toxicity

Toxicity data is not available for starch, carboxymethyl ether. Therefore, available aquatic toxicity data is provided for similar substance starch (CAS No. 9005-25-8).

Acute Studies

Table 2 lists the results of acute aquatic toxicity studies conducted on starch.

Table 2 Acute Aquatic Toxicity Studies on Starch (CAS No. 9005-25-8)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Orthopristis chrysoptera (pigfish)	96-h LC_{50}	>5,000	4	US EPA
Bairdiella chrysoura (silver perch)	96-h LC_{50}	>5,000	4	US EPA
Lagodon rhomboids (pinfish)	96-h LC_{50}	>5,000	4	US EPA

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Starch, carboxymethyl ether as a polysaccharide derivative is expected to be readily biodegradable. Therefore, it does not meet the screening criteria for persistence.

Starch, carboxymethyl ether is a polysaccharide derivative with an assumed high molecular weight (greater than 1,000,000 daltons) which limits its bioavailability to aquatic organisms. Therefore, it is not expected to bioaccumulate.

There are no chronic toxicity studies on starch, carboxymethyl ether. The acute LC_{50} values for read-across similar substance starch are >1 mg/L. Therefore, starch, carboxymethyl ether does not meet the screening criteria for toxicity.

Therefore, starch, carboxymethyl ether is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for starch, carboxymethyl ether.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Starch, carboxymethyl ether	9057-06-1	Not a PBT	No	No	No	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS, AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
dw	dry weight
EC	effective concentration

ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IMAP	Inventory Multitiered Assessment and Prioritisation
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

Starch, polymer with (chloromethyl)oxirane

This dossier on starch, polymer with (chloromethyl)oxirane presents the most critical studies pertinent to the risk assessment of the substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Starch, polymer with (chloromethyl)oxirane is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Starch, polymer with (chloromethyl)oxirane is an emulsifier, thickener and food additive. The substance is considered a polymer of low concern by NICNAS in an IMAP Tier 1 assessment. As a polymer of low concern, it is not expected to bioconcentrate or bioaccumulate. Based on its chemical structure, it is expected to be subject to degradation in the environment. Furthermore, it is not expected to exhibit toxicity to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Distarch glycerol

CAS RN: 58944-89-1

Molecular formula: $(C_3H_5ClO.Unspecified)x$- [This substance is a polymer.]

Molecular weight: 928.363 g/mol (monomer); polymer variable (UVCB)

Synonyms: Starch, polymer with (chloromethyl)oxirane; Starch, polymer with 2-(chloromethyl)oxirane;

3 PHYSICO-CHEMICAL PROPERTIES

No information is available.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for starch, polymer with (chloromethyl)oxirane.

NICNAS has assessed starch, polymer with (chloromethyl)oxirane in an IMAP Tier 1 assessment and considers it a polymer of low concern[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No studies on the environmental fate of starch, polymer with (chloromethyl)oxirane are available. However, the molecular structure, as identified in Pubchem, suggests it would be subject to hydrolysis and ring cleavage under environmental conditions. Thus, it is likely that starch, polymer with (chloromethyl)oxirane degrades readily. The high molecular weight of the polymer is expected to preclude or minimize bioaccumulation.

6 ENVIRONMENTAL EFFECTS SUMMARY

NICNAS has assessed starch, polymer with (chloromethyl)oxirane in an IMAP Tier 1 assessment and considers it a "polymer identified as a low concern to the environment."[2]. As a polymer of low concern, the substance is not expected to bioaccumulate or bioconcentrate. It may sorb to sediments and soil; however, it is not expected to exhibit toxicity to environmental receptors.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Data from a review of the molecular structure suggests that starch, polymer with (chloromethyl)oxirane will degrade in the environment. Thus, the substance does not meet the screening criteria for persistence.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=58944-89-1

[2] https://www.nicnas.gov.au/chemical-information/imap-assessments/how-chemicals-are-assessed/Low-concern-polymers.

Starch, polymer with (chloromethyl)oxirane is a high molecular weight polymer that is not expected to bioaccumulate. Thus, the substance does not meet the screening criteria for bioaccumulation.

There are no acute or chronic toxicity studies on starch, polymer with (chloromethyl)oxirane. However, as a polymer of low concern, it is not expected to exhibit toxicity to environmental receptors. Thus, starch, polymer with (chloromethyl)oxirane does not meet the screening criteria for toxicity.

The overall conclusion is starch, polymer with (chloromethyl)oxirane is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for starch, polymer with (chloromethyl)oxirane.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Starch, polymer with (chloromethyl)oxirane	58944-89-1	Not a PBT	No	Yes	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

SULFATED OLEIC ACID, POTASSIUM SALT

This dossier on sulfated oleic acid, potassium salt presents the most critical studies pertinent to the risk assessment of this substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the data published in the OECD-SIDS documents on aliphatic acids (OECD, 2014). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sulfated oleic acid, potassium salt is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sulfated oleic acid, potassium salt is a fatty acid salt. Fatty acids are amphiphilic compounds; in other words, each molecule has a hydrophilic, polar part (the carboxyl group) and a hydrophobic, nonpolar part (the hydrocarbon tail). The aliphatic acids category consists of C4-C22 aliphatic acids, also called fatty acids, and their salts (OECD, 2014).

As an aliphatic carboxylic acid salt, sulphated oleic acid, potassium salt will form the carboxylate anion or anions in the environment. It is expected to be readily biodegradable and to have generally low aquatic toxicity. AICIS has determined that this group of chemicals and their degradation products are unlikely to cause harm in the environment[1].

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Potassium; 1-carboxyheptadecan-8-yl sulfate

CAS RN: 68473-93-8

Molecular formula: $C_{18}H_{35}KO_6S$

Molecular weight: 418.6 g/mol

Synonyms: Sulfated oleic acid, monopotassium salt; Octadecanoic acid, 9(or 10)-(sulfooxy)-, monopotassium salt; 9(or 10)-(Sulfooxy) stearic acid potassium salt; Oleic acid, sulphated, potassium salt; 9(or 10)-(Sulfooxy) stearic acid monopotassium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=822-16-2

Table 1 Overview of the Physico-chemical Properties of Sulfated Oleic Acid, Potassium Salt*

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	-	PubChem
Melting Point	172.6 – 286.5 °C @ 101.3 kPa	-	OECD, 2014
Boiling Point	438.8 – 578.0°C @ 101.3 kPa	-	OECD, 2014
Density	1100 kg/m^3 (temperature not provided)**	-	USEPA, 2022
Vapour Pressure	1 x 10^{-10} – 1 x 10^{-12} Pa @ 25°C	-	OECD, 2014
Partition Coefficient (log K_{ow})	-2.17 – 4.13	-	OECD, 2014
Water Solubility	0.00332 g/L to 1000 g/L @ 25°C	-	OECD, 2014
Dissociation Constant (pKa)	~ 5	-	OECD, 2014
Viscosity	Not available	-	-

*Data provided for read-across category sodium and potassium salts, C6-C18 saturated

** Alternate CAS No. 68422-22-0

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sulfated oleic acid, potassium salt.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Sulfated oleic acid, potassium salt as a fatty acid salt is readily biodegradable. This substance has a low potential to bioaccumulate. It is poorly soluble in water and has high adsorption potential; thus, sediment and soil are expected to be the main targets for environmental distribution.

B. Biodegradation

No experimental data are available for sulfated oleic acid, potassium salt. Biodegradation studies or model estimations for single and multi-component aliphatic acids generally confirm that the extent of biodegradation observed in 28 days meets the ready biodegradability criterion (>60%). The aliphatic acids also undergo biodegradation under anaerobic conditions (OECD, 2014).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for sulfated oleic acid, potassium salt. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated organic carbon partition coefficient (K_{oc}) value from the molecular connectivity index (MCI) method is 7136 L/kg. Based on this K_{oc} value, if released to soil, sulfated oleic acid, potassium salt is expected to strongly adsorb to soil and have a low potential for mobility. If released to water, based on the K_{oc} value and its low water solubility, it is also expected to adsorb to suspended solids and sediment.

D. Bioaccumulation

There are no bioaccumulation studies on sulfated oleic acid, potassium salt. The BCF was estimated according to the BCFBAF model of EPISuite™ (USEPA, 2017). The estimated BCF ranged between 70.79 L/kg and 113 L/kg based on a log K_{ow} of 4.06 and the BCF ranged between 70.79 L/kg and 124.5 L/kg based on a log K_{ow} of 4.17. These BCFs correspond to a low bioaccumulation potential. Based on low water solubility and high adsorption coefficient, the substance is unlikely to be significantly bioavailable to aquatic organisms. As such, sulfated oleic acid, potassium salt is not expected to bioaccumulate in aquatic organisms.

6 ENVIRONMENTAL EFFECT SUMMARY

A. Summary

Sulfated oleic acid, potassium salt has low acute toxicity to aquatic organisms..

B. Aquatic Toxicity

<u>Acute Studies</u>

No aquatic toxicity studies are available for sulfated oleic acid, potassium salt. Data was obtained using read-across substances from the aliphatic acid category. The aliphatic acids share a common degradation pathway in which they are metabolized to acetyl-CoA or other key metabolites in all

living systems. Common biological pathways result in structurally similar breakdown products, and are, together with the physico-chemical properties, responsible for similar environmental behavior. Differences in metabolism or biodegradability of even and odd numbered carbon chain compounds or saturated/unsaturated compounds are not expected; even- and odd- numbered carbon chain compounds, and the saturated and unsaturated compounds are naturally occurring and are expected to be metabolized and biodegraded in the same manner. The acid and alkali salt forms of the homologous aliphatic acid are expected to have many similar physicochemical and toxicological properties when they become bioavailable; therefore, data read across is used for those instances where data are available for the acid form but not the salt, and vice versa. Sodium, potassium, magnesium, calcium and ammonium aliphatic acid salts contain the same chain length (or range) as a corresponding single component or Alkyl range or source based sponsored substance. As such, read across to the corresponding sponsored substances or supporting substances is reasonable. (OECD, 2014).

Table 3 lists the results of acute aquatic toxicity studies conducted on similar structural analogues to sulfated oleic acid, potassium salt. These values are consistent with chemical-specific values presented for sulfated oleic acid, potassium salt in the safety data sheet (SDS) for a product which contains the chemical (Halliburton, 2020).

Table 3 Acute Aquatic Toxicity Studies on Aliphatic Acids

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hr LC_{50}	54 (nominal)[a]*	-	OECD, 2014
Oryzias latipes	96-hr LC_{50}	125 (nominal)[b]*	-	OECD, 2014
Lepomis macrochirus	96-hr LC_{50}	23[c]*	-	OECD, 2014
Daphnia magna	48-hr EC_{50}	>100 (nominal)[d]*	-	OECD, 2014
Desmodesmus subspicatus	72-hr EC_{50}	25 (biomass) 41 (growth rate)[e]*	-	OECD, 2014
Desmodesmus subspicatus	72-hr EC_{50}	>100[d] (nominal)*	-	OECD, 2004

a – Fatty acids, C16-C18 and C18-unsaturated, sodium salts CAS No. 68424-26-0 (supporting substance for potassium and sodium salts)
b – Octadecanoic acid, sodium salt CAS No. 822-16-2
c – 9-Octadecanoic acid, (Z)-,potassium salt CAS No. 143-18-0
d – Octadecanedioic acid CAS No. 871-70-5
e – Fatty acids, C12-18, sodium salts CAS No. 91032-12-1

It should be noted that each of these values exceed the expected water solubility of the test substance.

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Based on data obtained from similar structural analogues, sulfated oleic acid, potassium salt is expected to be readily biodegradable; thus it does not meet the screening criteria for persistence..

Based on the estimated BCF values, sulfated oleic acid, potassium salt does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on sulfated oleic acid, potassium salt. However, the acute E(L)C_{50} values in similar structural analogues are >1 mg/L. Thus, the substance does not meet the screening criteria for toxicity.

The overall conclusion is that sulfated oleic acid, potassium salt is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sulfated oleic acid, potassium salt.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sulfated oleic acid, potassium salt	68473-93-8	Not a PBT	No	No	No	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern

DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L	litre
LC	lethal concentration
mg/L	milligrams per litre
mPa s	millipascal – second
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

MIXTURE OF DIMER/TRIMER FATTY ACIDS OF INDEFINITE COMPOSITION DERIVED FROM TALL OIL [FATTY ACIDS, TALL OIL]

This dossier on fatty acids, tall oil presents the most critical studies pertinent to the risk assessment of fatty acids, tall oil in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the Tall Oil Fatty Acid and Related Substances test plan and robust summaries submitted to the United States Environmental Protection Agency (USEPA) for the High Production Volume Information System (HPVIS) Chemical Challenge Program. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Fatty acids, tall oil is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Fatty acids, tall oil is a UVCB substance. Fatty acids are present in pine trees as glycerol esters; these fatty acids are saponified to sodium salts during the pulping process. These sodium salts are the major component of tall oil soap that is skimmed from spent pulping liquor and acidulated to form crude tall oil. Crude tall oil is then fractionally distilled at high temperatures under vacuum to yield several fractions, one of which is tall oil, fatty acids (HPVIS).

As a UVCB substance, the composition of a fatty acid, tall oil (CAS No. 61790-12-3) is: 1% palmitic acid, 2% stearic acid, 48% oleic acid, 35% linoleic acid, 7% conjugated linoleic acid, 4% other acids and 2% unsaponifiable matter (HPVIS).

Fatty acids, tall oil is readily biodegradable. It has a low potential for bioaccumulation and is of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Fatty acids, tall oil

CAS RN: 61790-12-3

Molecular formula: Variable

Molecular weight: Variable

Synonyms: Talllfettsuren (Harzsuregehalt <2 %);TALLOELFETTSAEUREN;TALL OIL L-1;Disproportionatedtalloilfattyacid;Fattyacids,tall-oil;tall;Talloilacids;Tall oil fatty acid

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Fatty acids, tall-oil

Property	Value	Klimisch score	Reference
Melting Point	NA		HPVIS
Boiling Point	NA		HPVIS
Vapour Pressure	NA		HPVIS
Partition Coefficient (log K_{ow})	4.2 – 7.4 @ pH 7.4	1	HPVIS
Water Solubility	0.0126 g/L @ 20°C	1	HPVIS

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for fatty acids, tall oil.

NICNAS has assessed fatty acids, tall oil in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Fatty acids, tall oil is readily biodegradable. It is insoluble and will likely strongly adsorb to soil or sediment. Substances in this category have a low potential for bioaccumulation.

B. Biodegradation

The results of biodegradation tests on fatty acids, tall oil are shown in Table 3.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=61790-12-3%2C+

Table 3 Biodegradation Tests on Fatty Acids, Tall Oil

Test	Results	Klimisch Score	Reference
OECD 301 D	50% after 7 days 56% after 28 days	1	HPVIS
OECD 301 F	84% after 28 days	1	HPVIS
Modified Sturm	74% after 28 days	1	HPVIS

The substance is readily biodegradable. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental studies are available for fatty acids, tall oil. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values for various surrogates of fatty acids, tall oil are presented in Table 4. These K_{oc} values along with the substance's insolubility indicates a strong potential for adsorption to soil and no mobility.

Table 4 K_{oc} Values for Surrogates of Fatty Acids, Tall Oil

Substance	K_{oc} [MCI estimate] (L/kg)	K_{oc} [log K_{ow} estimate]
Oleic acid	11,700	24,080
Linoleic acid	11,700	24,080

D. Bioaccumulation

No experimental data are available for fatty acids, tall oil. Using the bioconcentration factor/bioaccumulation factor (BCFBAF) model in EPISuite™ (USEPA, 2017), the estimated BCF for oleic and linoleic acid, the two major fatty acids, is 56.23 L/kg based on a regression based estimate. Based on this BCF value, this substance has a low potential for bioaccumulation.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Fatty acids, tall oil is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 5 lists the results of acute aquatic toxicity studies on fatty acids, tall oil.

Table 5 Acute Aquatic Toxicity Studies on Fatty Acids, Tall Oil

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LL_{50} NOEC	>1,000 (WAF) 1,000 (WAF)	1	HPVIS
Daphnia magna	48-hour EL_{50} NOEL	>1,000 (WAF) 1,000 (WAF)	1	HPVIS
Selenastrum capricornutum	72-hour EL_{50} NOEL	854.90 (WAF)* 500 (WAF)	1	HPVIS

*The 72-hour EL_{50} based on average specific growth rate was >1,000 mg/L with a corresponding $NOEL_r$ of 500 mg/L at 0-48 hours and 750 mg/L at 0-72 hours, indicating some inhibition (<50%) compared to the control.

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Fatty acids, tall oil is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on the estimated BCF value of 56.23 L/kg for two of the major components of fatty acids, tall oil, it does not meet the screening criteria for bioaccumulation.

For fatty acids, tall oil, the NOEC from an algal study and the acute EC_{50} values in fish, invertebrates and algae are greater than the water solubility of fatty acids, tall oil. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that fatty acids, tall oil is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for fatty acids, tall oil.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Fatty acids, tall oil	61790-12-3	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

HPVIS. U.S. EPA High Production Volume Information System (HPVIS): https://iaspub.epa.gov/oppthpv/public_search.html_page.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	bioconcentration factor/bioaccumulation factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EL	effect level
EU	European Union
HPVIS	High Production Volume Information System
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model

L/kg	litres per kilogram
LL	lethal loading
MCI	molecular connectivity index
mg/L	milligrams per litre
NOEC	no observed effect concentration
NOEL	no observed effect level
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	Water Accommodated Fraction

TETRAMETHYLAMMONIUM CHLORIDE

This dossier on tetramethylammonium chloride (TMAC) presents the most critical studies pertinent to the risk assessment of TMAC in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – TMAC was assessed as a tier 1 chemical for acute toxicity. This was based on aquatic toxicity studies for TMAC in fish along with the preponderance of data for read-across substance tetramethylammonium hydroxide (TMAOH) in invertebrates and algae indicating a classification of tier 1 (3 of 4 studies). TMAC was assessed as a tier 3 chemical for chronic toxicity based on a single aquatic toxicity study for TMAC in invertebrates. However, TMAC is determined to biodegrade in the environment very quickly suggesting chronic lab data would be less relevant than acute results. As a result, based on preponderance of data and biodegradation information, TMAC is classified overall as a **Tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

No biodegradation studies are available on TMAC; however, it is expected to be readily biodegradable based on tetramethylammonium hydroxide studies. TMAC has a moderate potential for adsorption to soil. It is not expected to bioaccumulate based on an octanol water partition coefficient (log Know) of <0.027. TMAC and its surrogate tetramethylammonium hydroxide (TMAOH) have moderate acute toxicity and high chronic toxicity concern for aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): N,N,N-trimethylmethanaminium chloride

CAS RN: 75-57-0

Molecular formula: $C_4H_{12}ClN$ or $(CH_3)_4NCl$

Molecular weight: 109.6 g/mol

Synonyms: Tetramethylammonium chloride; N,N,N-trimethylmethanaminium chloride; TMAC; tetramethylazanium; chloride

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Tetramethylammonium chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White hydroscopic powder with large solid lumps.	2	ECHA
Melting Point	268°C @ 101.3 kPa	1	ECHA
Boiling Point	Decomposition at 300°C before boiling point	1	ECHA
Density	1190 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	<1.6 x 10^{-8} Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	-1.6 @20°C	1	ECHA
Water Solubility	>1,000 g/L @ 20°C (pH 3.6)	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for TMAC.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

No biodegradation studies are available on TMAC; however, it is expected to be readily biodegradable based on TMAOH studies. TMAC has a moderate potential for adsorption to soil. It is not expected to bioaccumulate based on a log K_{ow} of <0.027.

B. Partitioning

TMAC is a quaternary ammonium salt, indicating that this compound will exist in the cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. As a salt, volatilisation from water or moist soil surfaces is not expected to be an important fate process. Likewise, based on its vapour pressure, volatilisation of TMAC from dry surfaces is also not expected to be an important fate process (PubChem).

Hydrolysis is not expected to be an important environmental fate process since this compound is a quaternary ammonium salt (PubChem).

C. Biodegradation

No biodegradation studies are available on TMAC. A 25% aqueous solution of TMAOH, a surrogate for TMAC, was readily biodegradable in an OECD 301B test. Degradation was 84% and 100% after 14 and 25 days, respectively (ECHA) [Kl. score = 1]. A 27.5% aqueous solution of TMAOH was readily biodegradable in an OECD 301C test. There was >90% degradation within 14 days (ECHA) [Kl. score = 2]. TMAOH was also readily biodegradable by adapted sludge under anaerobic conditions (ECHA) [Kl. score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

TMAC was tested in three different types of soil: loamy sand, sandy loam and clay soil. The mean K_{oc} for the three soils was 546 L/kg (ECHA). [Kl. score = 1]

If released to soil, based on this K_{oc} value, TMAC has a moderate potential for adsorption to soil. If released to water, based on this K_{oc} value along with its high water solubility, it is expected to also have a moderate potential for adsorption to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on TMAC. TMAC is not expected to bioaccumulate based on a log K_{ow} of <0.027 (ECHA) [Kl. score = 1].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

TMAC and its surrogate TMAOH have moderate acute toxicity and high chronic toxicity concern for aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on TMAC and its surrogate TMAOH.

Table 3 Acute Aquatic Toxicity Studies on TMAC and its surrogate TMAOH

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hr LC_{50}	462	2	ECHA
Daphnia magna	48-hr EC_{50}	3.6*	2	ECHA
Daphnia magna	48-hr EC_{50}	16.6*	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	115*	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50}	>301*	2	ECHA

*Test substance was TMAOH; values adjusted for TMAC (TMAC/TMAOH = 109/91).

Chronic Studies

An 11-day *Daphnia* reproduction study was conducted on TMAC. The NOEC was 0.03 mg/L (ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

TMAC is expected to be readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of <0.027, TMAC does not meet the screening criteria for bioaccumulation.

The lowest NOEC from the chronic aquatic toxicity studies on TMAC is <0.1 mg/L. Thus, TMAC does meet the criteria for toxicity.

The overall conclusion is that TMAC is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for TMAC.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Tetramethylammonium chloride	75-57-0	Not a PBT	No	No	No	No	No	Yes	1	3	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration

mg/L	milligrams per litre
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TMAC	tetramethylammonium chloride
TMAOH	tetramethylammonium hydroxide

TRIETHANOLAMINE

This dossier on triethanolamine presents the most critical studies pertinent to the risk assessment of triethanolamine in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Triethanolamine is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Triethanolamine, or TEA, is a viscous organic compound that is both a tertiary amine and a triol; a molecule with three alcohol groups. TEA is often used to facilitate lubricant formation in the drilling process.

It is readily degradable, does not persist in the environment and is of low toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2,2',2"-nitrilotriethanol

CAS RN: 102-71-6

Molecular formula: $C_6H_{15}NO_3$ or $(CH_2OHCH_2)_3N$

Molecular weight: 149.19 g/mol

Synonyms: Triethanolamine; 2,2',2"-nitrilotriethanol; 2,2',2"-nitrilotris[ethanol]; ethanol, 2,2',2"-nitrilotri- (8Cl); ethanol, 2,2',2"-nitrilotris- (9Cl); nitrilotriethanol; TEA; tris(beta-hydroxyethyl)amine; tris(2-hydroxyethyl)amine

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Triethanolamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless to pale-yellow liquid with an amine-like odour.	2	ECHA
Melting Point	20.5°C @ 101.3 kPa	2	ECHA
Boiling Point	336.1°C @ 101.3 kPa	2	ECHA

Property	Value	Klimisch score	Reference
Density	1120 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	Negligible	2	ECHA
Partition Coefficient (log K_{ow})	-1.9 @ 25°C [Experimental]	2	ECHA
Water Solubility	>1,000 g/L @ 20°C	2	ECHA
Viscosity	929.82 mPa s@ 20°C 203.28 mPa s @ 40°C	2	ECHA
Dissociation Constant (pKa)	7.86 @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for triethanolamine.

Based on an assessment of hazards, NICNAS identified the substance as a chemical of low concern to the environment (DoEE, 2017a). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Triethanolamine is readily biodegradable, and it has a low potential to bioaccumulate. Triethanolamine will not adsorb significantly to suspended solids and sediments in water and would be highly mobile in soil.

B. Biodegradation

Triethanolamine is readily biodegradable. In an OECD 301E test, there was 96% degradation after 19 days (ECHA). [Kl. score = 2]

Triethanolamine was completely degraded after incubation in municipal activated sludge for 1 or 5 days (West and Gonsior, 1996). The rate constants in all test batches for degradation and mineralisation were reported to be >0.359. Thus, triethanolamine can be considered to be readily biodegradable. [Kl. score = 2]

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017b).

C. Environmental Distribution

No experimental data are available for triethanolamine. Using KOCWIN in EPISUITE™ (U.S. EPA, 2017), the estimated K_{oc} value from log K_{ow} of -2.48 is 0.3046 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 10 L/kg.

If released to water, based on its low K_{oc} and high water solubility values, triethanolamine is likely to remain in water and not adsorb to sediment. It is also not expected to adsorb to soil, and, has the potential to be highly mobile.

D. Bioaccumulation

Triethanolamine has been tested in a bioconcentration flow-through fish (OECD 305) test using *Cyprinus carpio*. The BCF was determined to be <0.4 and <3.9 at triethanolamine concentrations of 2.5 and 0.25 mg/L, respectively (ECHA). [Kl. score = 2]

Based on the log K_{ow} (-2.48) and the calculated BCF, bioaccumulation is not to be expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Triethanolamine has low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on triethanolamine.

Table 3: Acute Aquatic Toxicity Studies on Triethanolamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-h LC_{50}	11,800	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Ceriodaphnia dubia	48-h EC_{50}	610	2	Warne and Schifko, 1999
Desmodesmus subspicatus	72-h EC_{50}	512 (neutralised) 216 (un-neutralised)	2	ECHA

Chronic Studies

In a 21-day *Daphnia* reproduction test, the NOEC for mortality is 16 mg/L, the NOEC for reproduction rate was 125 mg/L, and the NOEC for reproduction on the appearance of first offspring was 250 mg/L (Kuehn *et al.*, 1989). [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Triethanolamine is readily biodegradable; thus it does not meet the screening criteria for persistence.

The BCF values for triethanolamine in fish was <3.9; thus it does not meet the criteria for bioaccumulation.

The NOEC or EC_{10} values from chronic aquatic toxicity studies on triethanolamine is >0.1 mg/L. Thus triethanolamine does not meet the criteria for toxicity.

The overall conclusion is that triethanolamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for triethanolamine.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Triethanolamine	102-71-6	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy (DoEE). (2017a). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mm^2/s	square millimetres per second
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TEA	triethanolamine
USEPA	United States Environmental Protection Agency

TRIMETHYLAMMONIUM CHLORIDE

This dossier on trimethylammonium chloride does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies pertinent to the risk assessment of trimethylammonium chloride in its use in hydraulic fracturing fluids. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – trimethylammonium chloride is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Trimethylammonium chloride is the HCl salt of trimethylamine (N,N-dimethylmethanamine). Trimethylammonium chloride is expected to dissociate in aqueous media to the trimethylammonium cation and the Cl- anion. Based on information for trimethylamine, the trimethylammonium cation is expected to be readily biodegradable, has low potential to adsorb to soil and sediment, and is unlikely to bioaccumulate. There are no aquatic toxicity data on trimethylammonium chloride. Trimethylamine has low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): N,N-dimethylmethanamine chloride

CAS RN: 593-81-7

Molecular formula: $C_3H_{10}ClN$

Molecular weight: 95.6 g/mol

Synonyms: Trimethylammonium chloride; trimethylamine, hydrochloride; N,N-dimethanamine chloride; methanamine, N,N-dimethyl-, hydrochloride (9Cl)

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3 PHYSICO-CHEMICAL PROPERTIES

Trimethylammonium chloride is the hydrochloride salt of trimethylamine (N,N-dimethylmethanamine). Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Trimethylammonium chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline powder	2	ECHA

Property	Value	Klimisch score	Reference
Melting Point	273 – 278°C (pressure not reported)	2	ECHA
Boiling Point	Decomposition: >277°C (pressure not reported)	2	ECHA
Density	1040 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	Negligible	2	ECHA
Partition Coefficient (log K_{ow})	-2.25 @ 25°C	1	ECHA
Water Solubility	758 g/L @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for trimethylammonium chloride.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Trimethylammonium chloride is expected to dissociate in aqueous media to the trimethylammonium cation and the Cl^- anion. Based on information for trimethylamine, the trimethylammonium cation is expected to be readily biodegradable, has low potential to adsorb to soil and sediment, and is unlikely to bioaccumulate.

B. Biodegradation

No data are available on trimethylammonium chloride. However, trimethylamine (N,N-dimethymethanamine) was readily biodegradable in an OECD 301C test, with 92% degradation within 14 days (ECHA). [Kl. score = 2] If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for trimethylammonium chloride. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} value for trimethylamine (N,N-dimethylmethanamine) from log K_{ow} is 8.876 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 7.32 L/kg. Based on this estimated value, trimethylammonium chloride is expected to have very high mobility in soil. If released to water, based on the K_{oc} value and its high water solubility, it is also not expected to adsorb to suspended solids and sediment.

D. Bioaccumulation

No bioconcentration studies have been conducted on trimethylammonium chloride. Trimethylammonium chloride is not expected to bioaccumulate based on the experimental log K_{ow} of <-2.25 (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

There are no aquatic toxicity data on trimethylammonium chloride. Trimethylamine has a low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

No aquatic toxicity studies are available for trimethylammonium chloride. Table 3 lists the results of acute aquatic toxicity studies conducted on trimethylamine (N,N-dimethylmethanamine).

Table 3 Acute Aquatic Toxicity Studies on Trimethylamine (N,N-dimethylmethanamine)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Leuciscus idus	48-hr LC_{50}	25 (un-neutralised) 610 (neutralised)	2	ECHA
Daphnia magna	48-hr EC_{50}	139.95	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50} EC_{10}	150 (growth rate) 90.6 (biomass) 86 (growth rate) 42.6 (biomass)	2	ECHA

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Trimethylammonium chloride is expected to be readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of <-2.25 trimethylammonium chloride does not meet the screening criteria for bioaccumulation.

There are no aquatic toxicity studies on trimethylammonium chloride. The acute EC_{50} values of trimethylamine (N,N-dimethylmethanamine) are >1 mg/L for fish, invertebrates and algae. Thus, trimethylammonium chloride is not expected to meet the screening criteria for toxicity.

The overall conclusion is that trimethylammonium chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for trimethylammonium chloride.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Trimethylammonium chloride	593-81-7	Not a PBT	No	No	No	No	No	No	1	No data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model

kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

ULEXITE

This dossier on ulexite presents the most critical studies pertinent to the risk assessment of ulexite in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Ulexite is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Ulexite is a sodium-calcium-hydroborate and, like other borates, is a structurally complex mineral. It is composed of hydrogen (3.98 %), sodium (5.67 %), calcium (9.89 %), boron (13.34 %), and oxygen (67.12 %), alternatively expressed as Na_2O (7.65 %), CaO (13.84 %), H_2O (35.57 %), and B_2O_3 (42.95 %) (Gulensoy & Kocakerim, 1977; Webmineral).

The boron concentration of ulexite is commercially significant because boron compounds are used in producing materials for many branches of industry. Boron is primarily used in the manufacturing of fiberglass along with heat resistant borosilicate glasses such as traditional Pyrex, car headlights, and laboratory glassware. Boron and its compounds are also common ingredients in soaps, detergents, and bleaches, which contributes to the softening of hard water by attracting the calcium ions.

In coal seam gas applications, the hydraulic fracturing fluid primarily consists of sand, water and guar gum. Boric acid or borates are commonly added to this guar gum slurry to increase its viscosity and provide stability (Stringfellow et al. 2014).

Boron is an inorganic, elemental compound and can therefore not be biodegraded by micro-organisms or other biotic-related processes. It does not bioaccumulate in the aquatic environment. Boron is of a low toxicity concern to aquatic organisms. Although boron is required by plants at low concentrations, at high concentrations it is toxic. In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron. The phytotoxicity of boron is dependent on the plant species and soil type (DoEE, 2017).

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name: Sodium-calcium pentaborate octahydrate

CAS RN: 1319-33-1

Molecular formula: $(NaCaB_5O_6(OH)_6{\cdot}5H_2O)$

Molecular weight: 405 g/mol

Synonyms: Ulexite; sodium-calcium pentaborate octahydrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Commercially Available Ulexite

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, granular, ground, or powder form	4	Etimine USA, Inc. (2016)
Melting Point	870°C	4	Etimine USA, Inc. (2016)
Boiling Point	Not Applicable	-	-
Bulk Density	1,410 to 1,500 kg/m^3	4	Etimine USA, Inc. (2016)
Water solubility	26.67% as dissolved Ulexite @ 25°C by weight of solution	4	American Borate Company (2016)

Ulexite is a naturally-occurring mineral that is slightly soluble in water. Limited measured data are available for ulexite. In a study investigating the relative rates of boron from soluble and controlled-release boron fertilizers, ulexite showed releases of boron of 20% in just under 10 weeks; 40% in approximately 25 weeks; 60% by 40 weeks; and 80% by 60 weeks (Broschat, 2008). In the environment, borates will dissociate and/or hydrolyse to release boron as boric acid [$B(OH)_3$ (also formulated as H_3BO_3)] and/or borate anions. Therefore, the information presented within this dossier is for boron (CAS No. 7440-42-8).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ulexite.

NICNAS has assessed ulexite in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=1319-33-1%2C+

5 ENVIRONMENTAL FATE SUMMARY

Boron is found almost exclusively in the environment in the form of boron-oxygen compounds, which are often referred to as borates. In the environment, borates and compounds of boric acid will dissociate and/or hydrolyse to form the same boron species. For example, when borax dissolves in dilute solutions, it dissociates into Na+ ions and the tetraborate anion ($B_4O_5(OH)_4^{2-}$). Boric acid ($B(OH)_3$) is formed following acid catalysed hydrolysis of the tetraborate anion. Under alkaline conditions, dilute solutions of the tetraborate anion depolymerise rapidly to the mononuclear borate anion ($B(OH)_4^-$) (DoEE, 2017).

Boron is an inorganic, elemental compound and can therefore not be biodegraded by micro-organisms or other biotic-related processes (ECHA).

The WHO (1998) review of boron noted that highly water soluble materials are unlikely to bioaccumulate to any significant degree and that borate species are all present essentially as undissociated and highly soluble boric acid at neutral pH. The available data indicate that both experimental data and field observations support the interpretation that borates are not significantly bioaccumulated (ECHA).

Bioconcentration factors of <0.1 to 10.5 L/kg have been reported from laboratory tests of fish and oysters (Thompson et al. 1976). Saiki et al. (1993) measured boron levels in aquatic food chains and observed the highest concentrations of boron in detritus and filamentous algae. Invertebrates and fish had lower concentrations, indicating that bioaccumulation was not occurring. Based on these data, boron does not bioaccumulate in the aquatic environment (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

There are no mammalian or aquatic toxicity studies on ulexite. Toxicity for boron is provided within this section.

Boron is of a low toxicity concern to aquatic organisms. Although boron is required by plants at low concentrations, at high concentrations it is toxic. In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron. The phytotoxicity of boron is dependent on the plant species and soil type (DoEE, 2017).

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on boron.

Table 3 Acute Aquatic Toxicity Studies on boron[1]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
P. promelas	4 day LC_{50}	79.7 mg B/L	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Freshwater invertebrates	48-hr LC_{50}	64 to >544 mg/B/L	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	52.4 mg/B/L	2	ECHA

1/ CAS No. 7440-42-8

Chronic Studies

Table 4 lists the results of chronic aquatic toxicity studies on boron.

Table 4 Chronic Aquatic Toxicity Studies on boron[1]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Micropterus salmoides	4d-EC10	36.8 mg B/L	2	ECHA
Oncorhynchus mykiss	long term NOEC-LOEC	19.2. mg/B/L	2	ECHA
Brachydanio rerio	long term NOEC-LOEC	36.mg/B/L	2	ECHA
Pimephales promelas	long term NOEC-LOEC	21.3 mg/B/L	2	ECHA
Daphnia magna	NOEC	13.9 mg/B/L	2	ECHA
Hyalella azteca	NOEC	6.3 mg/B/L	2	ECHA
Chironomus riparius	NOEC	20.1 mg/B/L	2	ECHA
Brachionus calyciflorus	NOEC	24.6 mg/B/L	2	ECHA
Lampsilis siliquoidea	NOEC	30 mg/B/L	2	ECHA

1/ CAS No. 7440-42- 8 for boron

ANZG has developed a water quality guideline for boron (ANZG, 2021). Very high reliability default guideline values (DGVs) for (dissolved) boron in freshwater were derived from 22 chronic (long-term) toxicity data, comprising eight fish, two amphibians, three crustaceans, one bivalve, three macrophytes, one green microalga, three diatoms and one blue–green alga. The DGVs for 99, 95, 90 and 80% species protection are 340 µg/L, 940 µg/L, 1,500 µg/L and 2,500 µg/L, respectively. The 95% species protection level for boron in freshwater (940 µg/L) is recommended for adoption in the assessment of slightly-to-moderately disturbed ecosystems.

C. Terrestrial Toxicity

Relevant and reliable chronic no-effects values were identified for thirty-nine terrestrial species or microbial processes. No-effect levels for dissolved boron ranged between 7.2 mg B/kg soil dw and 86.7 mg B/kg soil dw. The plant Zea mays was the most sensitive trophic level. The least sensitive species was the nematode C.elegans. A Species Sensitivity Distribution (SSD) has been developed for

the assessment of boron in the terrestrial compartment, using the reliable species-specific chronic toxicity effect levels that have been generated in various research studies. (ECHA)[KI Score = 2).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Ulexite is a naturally-occurring mineral. For the purposes of this PBT assessment, the persistence criteria is not considered applicable to this inorganic substance.

Bioaccumulation is not applicable to naturally-occurring minerals, such as ulexite. Although boron is slowly released from ulexite, limited data indicate that bioaccumulation is not significant in aquatic and terrestrial food chains. Thus, it does not meet the criteria for bioaccumulation.

There are no mammalian or aquatic toxicity studies on ulexite. Ulexite, being a slightly water-soluble mineral, is not expected to be bioavailable. The lowest chronic toxicity value for boron is >0.1 mg/L. The acute E(L)C_{50} values for boron is >1 mg/L. Thus, based on boron, ulexite does not meet the criteria for toxicity.

Therefore, ulexite is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ulexite.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Ulexite	1319-33-1	Not a PBT	No	No	NA	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

American Borate Company (2016). Technical specifications on Ulexite 45 micron ground. Available at: http://www.americanborate.com/media/19191/ulexite-1319-33-1-2016-technical-specification.pdf.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
LOEC	lowest observed effect concentration
mg/B/L	milligram boron per litre
NOEC	no observed effect concentration
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

VINYLAMIDE/VINYL SULFONATED POLYMER

This dossier on vinylamide/vinyl sulfonated polymer presents the most critical studies pertinent to the risk assessment of vinylamide/vinyl sulfonated polymer in its use as a cement additive chemical. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion: Vinylamide/vinyl sulfonated polymer is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

High molecular weight copolymers based on vinyl sulfonate, and vinyl amide show high performances in the demanding requirements for enhanced oil recovery (EOR) flooding processes. These synthetic anionic polymers are of low water solubility and exhibit low toxicity. They are biocompatible and used in the pharmaceutical, medical and oil recovery industries.

Due to their large size and negative charge, anionic polymers cannot cross biological membranes. The polymers therefore cannot cause intracellular toxic effects or bioaccumulate (Boethling and Nabholz, 1997). On this basis, anionic polymers generally have low toxicity to fish and aquatic invertebrates. However, anionic polymers may have moderate toxicity to algae because they have the potential to over-chelate Ca^{2+} and Mg^{2+} cations which are nutrients needed for growth (Boethling and Nabholz, 1997). This mode of toxic action is directly related to the carbon distance between acid functional groups on the polymer backbone. The highest toxicity occurs when the acid is on alternating carbons of the polymer backbone (DoEE, 2017).

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1-Propanesulfonic acid, 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-, ammonium salt (1:1), polymer with 2-propenamide

CAS RN: 110897-64-8

Molecular formula: $(C_7H_{13}NO_4S.C_3H_5NO.H_3N)_x$ [This substance is a polymer.]

Molecular weight: 295 g/mol (monomer); polymer variable (UVCB)

Synonyms: Vinylamide/vinyl sulfonated polymer;

3 PHYSICO-CHEMICAL PROPERTIES

No chemical-specific information is available. High molecular weight polymers increase the solution viscosity for EOR flooding processes. Molecular weights in this group range from 10,000 g/mol to 10,000,000 g/mol (Scott et al., 2020).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for vinylamide/vinyl sulfonated polymer.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No experimental data are available vinylamide/vinyl sulfonated polymer.

Polymers with a molecular weight greater than 1,000 g/mol generally have a negligible vapor pressure, which indicates that the chemical is likely to exist solely as particulate matter in the atmosphere. As particulate matter, atmospheric oxidation is not expected to be a significant route of environmental removal. Likewise, volatilization from water or moist soil is not expected to occur at an appreciable rate (USEPA, 2013).

Anionic polymers of this type are expected to be water soluble based on their predominately hydrophilic structure. In water, they are expected to dissociate to release similar high molecular weight polyanions based on the typical acidity of the functional group moieties present in each polymer. They are expected to partition onto natural colloids in surface waters and in soil (DoEE, 2017). However, due to large size and weight parameters, these materials may still have low mobility in soil (USEPA, 2013).

Synthetic anionic polymers are not expected to undergo rapid degradation (DoEE, 2017). However, due to the large size, they are typically of low concern for bioconcentration. Polymers with a number average molecular weight (NAMW) greater than 1,000 g/mol cannot cross biological membranes (Boethling and Nabholz 1997).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Aquatic Toxicity

No ecotoxicity data was identified for vinylamide/vinyl sulfonated polymer. Information on Anionic Polymers Group (DoEE, 2017) is provided below.

"High molecular weight anionic polymers (including water-soluble polyanions) generally have low toxicity to fish and aquatic invertebrates. These polymers cannot be absorbed across biological membranes in aquatic organisms, and therefore toxicity only occurs through indirect effects such as chelation of essential nutrients. This is supported by median lethal concentration (LC50) values available for anionic polymers which are typically greater than 100 mg/L (Boethling and Nabholz 1997).

Water soluble or dispersible anionic polymers may be moderately toxic to algae because they have the potential to over-chelate Ca_{2+} and Mg^{2+} cations which are essential nutrients needed for growth (Boethling and Nabholz 1997). Toxicity by this mechanism is directly related to the carbon distance between acid functional groups. The highest toxicity occurs when the acid is on alternating carbons of the polymer backbone and homopolymers of acrylic acid generally have the highest indirect toxicity to algae for this reason (Boethling and Nabholz 1997).

The polymers in this group may have some potential to chelate Ca^{2+} and Mg^{2+} cations if they have a significant number of repeating acid units in the polymer structure. However, the toxicity to algae is likely to be reduced under most circumstances due to the presence of background concentrations of calcium ions in most applications, which will bind to the chelating residues in the polymers before they are released to the environment. Even under optimal conditions for toxicity of homopolymers of acrylic acid, the measured median effect concentration (EC50) values for these indirect toxicity effects to algae are greater than 3 mg/L (Boethling and Nabholz 1997)."

B. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Vinylamide/vinyl sulfonated polymer is not expected to be biodegradable. Thus, it meets the criteria for persistence.

Vinylamide/vinyl sulfonated polymer is not expected to bioaccumulate. Polymers with a NAMW greater than 1,000 g/mol cannot cross biological membranes (Boethling and Nabholz 1997). Thus, it does not meet the screening criteria for bioaccumulation.

No aquatic toxicity studies are available for vinylamide/vinyl sulfonated polymer. It is expected to be a low concern of toxicity to aquatic organisms because of its low potential for bioavailability. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that vinylamide/vinyl sulfonated polymer is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for vinylamide/vinyl sulfonated polymer.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Vinylamide-vinyl sulfonated polymer	110897-64-8	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Boethling RS, and Nabholz JV 1997, 'Environmental assessment of polymers under the US Toxic Substances Control Act', in Hamilton J and Sutcliffe R (eds), Ecological assessment of polymers: strategies for product stewardship and regulatory programs, Van Nostrand Reinhold, New York, USA, pp 187-234.

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Scott, Alison J., Laura Romero-Zeron and Alexandar Penlidis. (2020). Evaluation of Polymeric Materials for Chemical Enhanced Oil Recovery. Processes 2020, 8, 361; doi:10.3390/pr8030361

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

VINYLIDENE CHLORIDE/METHYLACRYLATE COPOLYMER

This dossier on vinylidene chloride/methylacrylate copolymer presents the most critical studies pertinent to the risk assessment of vinylidene chloride/methylacrylate copolymer in its use in hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion: Vinylidene chloride/methylacrylate copolymer is a polymer of low concern. Therefore, it is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Vinylidene chloride/methylacrylate copolymer is the copolymer of methyl acrylate and vinylidene chloride. No studies on the environmental fate of vinylidene chloride/methylacrylate copolymer are available. Synthetic non-ionic polymers are not expected to undergo rapid degradation. However, based largely on its high molecular weight, the substance is not expected to bioaccumulate or bioconcentrate. It is of low toxicity to environmental receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1,1-dichloroethene;methyl prop-2-enoate

CAS RN: 25038-72-6

Molecular formula: $(C_2H_2Cl_2)_x(C_4H_6O_2)_y$ [This substance is a polymer.]

Molecular weight: 183.03 g/mol (monomer); polymer assumed to be > 1000 g/mol (NICNAS, 2017a)

Synonyms: vinylidene chloride/methylacrylate copolymer; methyl acrylate-vinylidene chloride copolymer; 2-propenoic acid, methyl ester, polymer with 1,1-dichloroethene

3 PHYSICO-CHEMICAL PROPERTIES

No chemical-specific information is available. Vinylidene chloride/methylacrylate copolymer is a non-ionic synthetic polymer. It is formed by addition polymerisation, which typically affords high molecular weight polymers with stable saturated carbon-chain backbones. Water solubility is expected to be low based on the predominantly hydrophobic structure of the substance.

As noted, no information is available regarding the molecular weight and the percentage of low molecular weight (LMW) species in this polymer. However, synthetic addition polymers of this type are generally high to very high molecular weight species. It is assumed for this polymer that the number average molecular weight (NAMW) is greater than 1,000 daltons (Da) with an insignificant percentage of LMW species (DoEE, 2017).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No

conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for vinylidene chloride/methylacrylate copolymer.

NICNAS has assessed vinylidene chloride/methylacrylate copolyme in an IMAP Tier 1 assessment and considers it a polymer of low concern[1] . In addition, based on an assessment of human health and environmental hazards, NICNAS also identified vinylidene chloride/methylacrylate copolymer as a chemical of low concern to the environment (NICNAS, 2017 and DoEE, 2017). Chemicals of low concern are unlikely to have adverse environmental effects or be a concern to human health if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

No experimental data are available for vinylidene chloride/methylacrylate copolymer.

Polymers with a molecular weight greater than 1,000 g/mol generally have a negligible vapor pressure, which indicates that the chemical is likely to exist solely as particulate matter in the atmosphere. As particulate matter, atmospheric oxidation is not expected to be a significant route of environmental removal. Likewise, volatilization from water or moist soil is not expected to occur at an appreciable rate (USEPA, 2013).

Non-ionic polymers such as vinylidene chloride/methylacrylate copolymer are not expected to be highly soluble in water based on its predominantly hydrophobic structure. If discharged to the aquatic environment, this polymer is expected to partition to soil or sediment. It is not expected to be highly mobile if released to the soil compartment (Beothling and Nabholz 1997).

Synthetic non-ionic polymers are not expected to undergo rapid degradation (NICNAS, 2017a). However, the high molecular weight of the polymer is expected to preclude or minimize bioaccumulation. Polymers with a number average molecular weight (NAMW) greater than 1,000 g/mol cannot cross biological membranes (Boethling and Nabholz 1997).

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=25038-72-6

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Aquatic Toxicity

No ecotoxicity data was identified for vinylidene chloride/methylacrylate copolymer. Information on Non-Ionic Polymers Group (DoEE, 2017) is provided below.

> *"Non-ionic polymers with low water solubility, such as the methyl acrylate-vinylidene chloride copolymer, generally have low toxicity to aquatic life (Beothling and Nabholz 1997). Insoluble non-ionic polymers have low bioavailability and their adverse effects result from physical. effects such as occlusion of respiratory organs (e.g. the gills of fish). These adverse effects occur only at very high loading levels in water (Beothling and Nabholz 1997).*
>
> *Water soluble or dispersible non-ionic polymers, such as polyacrylamide, are also typically of low concern for ecotoxicity. Non-ionic polymers with NAMW greater than 1 000 cannot be absorbed across biological membranes in aquatic organisms, and therefore toxicity only occurs through indirect effects such as chelation of essential nutrients (Beothling and Nabholz 1997). However, the structure of polyacrylamide suggests that it will have low potential to act by this mode of action. This is further supported by median effective concentration (EC50) and median lethal concentration (LC50) values available for other water soluble or dispersible non-ionic polymers, which are greater than 100 mg/L (Beothling and Nabholz 1997).*
>
> *Water soluble or dispersible polymers with NAMW less than 1 000 Da, or significant levels of LMW substances and trapped monomers, are of potential concern because of their increased bioavailability. However, this assessment was conducted assuming that the polymers in this group have NAMW greater than 1 000 Da and the percentage of LMW species is low."*

B. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Vinylidene chloride/methylacrylate copolymer is not expected to be biodegradable. Thus, it meets the criteria for persistence.

Vinylidene chloride/methylacrylate copolymer is not expected to bioaccumulate. Polymers with a NAMW greater than 1,000 g/mol cannot cross biological membranes (Boethling and Nabholz 1997). Thus, it does not meet the screening criteria for bioaccumulation.

No aquatic toxicity studies are available for vinylidene chloride/methylacrylate copolymer. It is expected to be a low concern of toxicity to aquatic organisms because of its low potential for bioavailability. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that vinylidene chloride/methylacrylate copolymer is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for vinylidene chloride/methylacrylate copolymer.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Vinylidene chloride/methylacrylate copolymer	25038-72-6	Not a PBT	No	Yes	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Boethling RS, and Nabholz JV 1997, 'Environmental assessment of polymers under the US Toxic Substances Control Act', in Hamilton J and Sutcliffe R (eds), Ecological assessment of polymers: strategies for product stewardship and regulatory programs, Van Nostrand Reinhold, New York, USA, pp 187-234.

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

European Chemicals Agency [ECHA]. (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

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United States Environmental Protection Agency (USEPA). (2013). Interpretive Assistance Document for Assessment of Polymers: Sustainable Futures Summary Assessment. June 2013.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency

EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
NAMW	number average molecular weight
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Walnut hulls

Nut hulls

Almond Hulls

Vegetable Fibre

Wood Fibre

This dossier on walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre presents the most critical studies pertinent to the risk assessment of these substance in their use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are classified as **tier 1** chemicals and require a hazard assessment only.

1 BACKGROUND

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are used to control lost circulation in water oil base drilling fluids. They may be utilized intact or in pill form with fibrous flake material.

The predominant degradation pathway for woody materials in the environment is expected to be microbial decomposition, whereby extracellular enzymes secreted by bacteria and fungi breakdown or otherwise transform the biopolymers in plant cell walls. Such decomposition processes are ubiquitous in the environment and are an important part of the biogeochemical carbon cycle (DoEE, 2017a).

Woody materials that have not been chemically treated are not considered to be directly toxic to biota.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Not applicable

CAS RN: Not applicable

Molecular formula: Not applicable

Molecular weight: Not applicable

Synonyms: Not applicable

3 PHYSICO-CHEMICAL PROPERTIES

Nut shells differ chemically. Walnut shells have approximately 10.6% extractives, 30.1% lignin, and 49.7% polysaccharides, whereas almond shells have 5.7% extractives, 28.9% lignin, and 56.1% polysaccharides. The polysaccharide composition of walnut and almonds as the glucose/xylose ratio is 1.12. Walnut and almond shells have a syringyl (S) and guaiacyl (G) lignin ratio of 1.6 and 1.0. Wood and vegetable fibres are natural composite structures in which cellulose fibrils are held together by lignin and hemicellulose. The major constituents of wood fibres are lignin, cellulose, hemicellulose, and extractives. Each of these components contributes to fibre properties, which ultimately impact product properties.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is not listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre.

Based on an assessment of environmental hazards, NICNAS identified wood products (which contains wood fibre, walnut hulls, nut hulls and natural fibres) as a chemical of low concern to the environment (DoEE, 2017b). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are biodegradable, are not expected to bioaccumulate, and in the terrestrial environment are expected to become part of the organic carbon pool in the soil where it will act as an important physical and chemical constituent.

B. Biodegradation

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are expected to degrade over time under typical environmental conditions.

Wood and other plant based materials are biodegraded by bacteria and fungi, over sometimes very long (i.e. 1 000 year) time scales, with wood being an important carbon source in terrestrial ecosystems (e.g. Blanchette 2000; Wetzel 2001). The rates of decay and the biochemical pathways involved in wood decay are dependent on the environment in which the wood occurs, with decomposition possible in both anoxic and oxic environments (DoEE, 2017a).

C. Environmental Distribution

Wood products distributed in the terrestrial environment are expected to become part of the organic carbon pool in the soil where it will act as an important physical and chemical constituent. The materials in this group are transportable into water bodies either through indirect pathways where they can be entrained in runoff, or direct pathways as a result of spillage. In the aquatic environment, wood products can be viewed as particulate organic matter and are expected to become part of the aquatic carbon cycle. Decay rates for wood products in aquatic ecosystems are highly variable, with woody materials degrading before they reach the sediments in some aquatic ecosystems and being preserved for centuries in others (DoEE, 2017a).

D. Bioaccumulation

Nut shells are not bioaccumulative.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are of low acute toxicity concern to aquatic organisms.

Woody materials that have not been chemically treated are not considered to be directly toxic to biota. Nevertheless, organic matter such as woody materials can act as non-toxic stressors that have direct or indirect effects on aquatic ecosystems. However, in the aquatic environment, wood products can be viewed as particulate organic matter and are expected to become part of the aquatic carbon cycle (DoEE, 2017a).

B. Aquatic Toxicity

No data are available.

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are expected to biodegrade.

They do not meet the screening criteria for bioaccumulation.

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are not expected to exhibit aquatic toxicity.

Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for walnut hulls, nut hulls, and almond hulls.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Walnut hulls, nut hulls, almond hulls, vegetable fibre and wood fibre	NA	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA]. (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017a) Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report Appendices A, B, C, D, F, and G prepared by the Chemicals and Biotechnology Assessments Section (CBAS) in the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

DoEE. (2017b). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SGG	Synthetic Greenhouse Gases

WATER

This dossier on water presents the most critical studies pertinent to the risk assessment of water in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Water is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Water is an inorganic, transparent, tasteless, odorless, and nearly colorless chemical substance, which is the main constituent of Earth's hydrosphere and the fluids of all known living organisms (in which it acts as a solvent). It is vital for all known forms of life, even though it provides no calories or organic nutrients. Its chemical formula is H_2O, meaning that each of its molecules contains one oxygen and two hydrogen atoms, connected by covalent bonds.

Water is present as the dominant constituent of aqueous solutions and slurries used in hydraulic fracturing operations. Water is essential for all life and is not considered to be an ecotoxicological hazard (DoEE, 2017).

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Oxidane, water

CAS RN: 7732-18-5

Molecular formula: H_2O

Molecular weight: 18.015 g/mol

Synonyms: hydroxic acid, hydroxylic acid, and hydrogen hydroxide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Water

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	clear liquid	-	PubChem
Melting Point	0°C @ 101.3 kPa	-	PubChem
Boiling Point	100°C @ 101.3 kPa	-	PubChem
Partition Coefficient (log P_{ow})	Not Applicable	-	PubChem

Property	Value	Klimisch score	Reference
Density	997 kg/m3 @ 20℃	-	PubChem
Water Solubility	Not Applicable	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for water.

Based on an assessment of hazards, NICNAS identified the substance as a chemical of low concern to human health and the environment (NICNAS, 2017 and DoEE, 2017a). Chemicals of low concern are considered to have a low likelihood of causing adverse human health effects should an exposure occur and are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Water is absolutely essential to all life. The protoplasm of most living cells contains about 80% water. Most of the earth's surface is covered with water. The most striking feature of the earth is the extensive hydrosphere, lacking from neighboring planets. 97.22% of earth's water is captured in oceans, with approximately 2% of water locked up in polar icecaps and glaciers. Water found in land, including surface and groundwater, makes up <1% of the earth's water resources. Groundwater represents more than 97% of the usable freshwater resources and is a major source of replenishment for surface water. Water resources are renewable but finite and scarce. Only freshwater flowing through the solar-powered hydrological cycle is renewable (PubChem).

Water which evaporates from the surface of oceans, fresh watercourses, and vegetation is carried in the air to be precipitated as rainfall or snow. The molecules of water vapor in air are pure water; falling raindrops formed by their condensation are saturated with nitrogen, oxygen and other atmospheric gases (PubChem).

6 ENVIRONMENTAL EFFECTS SUMMARY

Water is essential for all life and is not considered to be an ecotoxicological hazard (DoEE, 2017b).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The biodegradation endpoint is not relevant for water. As such, water does not meet the screening criteria for persistence.

Bioconcentration studies are not relevant for water. Therefore, water does not meet the screening criteria for bioaccumulation.

Water may exert adverse effects depending on the ionic nature of dissolved inorganic substances in the aqueous matrix. However, as a separate chemical entity, water does not meet the screening criteria for toxicity.

The overall conclusion is that water is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for water.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Oxidane (Water)	7732-18-5	Not a PBT	No	No	NA	No	NA	No	NA	NA	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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PubChem. National Institutes of Health. National Library of Medicine National Center for Biotechnology Information. https://pubchem.ncbi.nlm.nih.gov/

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency

EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

XANTHAN GUM

This dossier on xanthan gum does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies pertinent to the risk assessment of xanthan gum in its use in drilling muds. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Xanthan gum is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Xanthan gum is a high molecular weight polysaccharide produced by the bacterium *Xanthomonas campestris*. It may be degraded, but it is not readily biodegradable. Due to its high molecular weight, it is not expected to be bioavailable and thus not bioaccumulate. Xanthan gum is not acutely toxic.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Xanthan Gum

CAS RN: 11138-66-2

Molecular formula: $C_{35}H_{49}O_{29}$ (as the monomer)

Molecular weight: 2 x 10^6 g/mol (Dintzis *et al.*, 1970)

Synonyms: Xanthan gum, gum xanthan, corn sugar gum

3 PHYSICO-CHEMICAL PROPERTIES

No specific data were located. Xanthan gum is a cream-colored, odorless, free-flowing powder. Xanthan gum has unique physical properties that have resulted in applications in the food, cosmetic, pharmaceutical, and oil and gas industry. Xanthan gum shows pseudoplasticity of solution, minimal change of viscosity over a wide range of temperatures, solubility and stability in both acid and alkaline solutions, viscosity stability over a wide pH range, and suspending properties for hard-to-suspend solids (Rocks, 1971).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for xanthan gum.

NICNAS has assessed sodium citrate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health[1] .

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Xanthan gum is a high molecular weight polysaccharide gum produced by the bacterium *Xanthomonas campestris*. It is highly soluble. Studies have shown that xanthan gum may be degraded by some micro-organisms, but it is not readily biodegradable. It is not expected to bioaccumulate due to its large molecular weight.

No biodegradation studies were identified. Xanthan gum is a highly stable polysaccharide that is not easily degraded by most micro-organisms (Cadmus *et al.*, 1982). The stability of xanthan gum may be affected when soil organisms at high concentrations are in contact with it for one month (Cadmus *et al.*, 1982). These investigators were also able to isolate certain strains of bacteria isolated from sewage sludge and soil that released enzymes that could degrade xanthan gum (Cadmus *et al.*, 1982). These findings suggest that xanthan gum may be degradable, but not readily biodegradable.

Xanthan gum is a high molecular weight polysaccharide (2,000,000 daltons). Due to its large molecular weight, it is not expected to be bioavailable. Therefore, xanthan gum is not expected to bioaccumulate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Xanthan gum is not expected to pose an appreciable hazard to environmental receptors due principally to its large molecular weight and associated reduced bio availability.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=11138-66-2

B. Aquatic Toxicity

Limited studies are available on xanthan gum. Xanthan gum is a high molecular weight polysaccharide (2,000,000 daltons), which due to its size, is not expected to be bioavailable. Hence, xanthan gum is expected to be non-toxic to aquatic organisms.

A 96-hour LC_{50} value for fish (Rainbow Trout) has been reported to be 420 mg/ (DoEE, 2017).

C. Terrestrial Toxicity

No studies are available.

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

There are no biodegradation studies on xanthan gum. Xanthan gum is a highly stable polysaccharide that is not easily degraded by most micro-organisms, although there are some bacterial strains that can degrade this polysaccharide. Xanthan gum is expected to be degradable but is unlikely to be readily biodegradable. Therefore, it is expected to meet the screening criteria for persistence.

Xanthan gum is a high molecular weight polysaccharide (2,000,000 daltons), which due to its size, is not expected to be bioavailable. Therefore, xanthan gum is not expected to meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on xanthan gum. The acute LC_{50} values are >1 mg/L in fish. Xanthan gum is expected to be non-toxic to aquatic organisms because its high molecular weight will limit its bioavailability.

The overall conclusion is that xanthan gum is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for xanthan gum.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Xanthan gum	11138-66-2	Not a PBT	No	No	Yes	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Cadmus, M.C, L. K. Jackson, K. A. Burton, R. D. Plattner, and M. E. Slodki. (1982). Biodegradation Of Xanthan Gum By Bacillus Sp. Applied and Environmental Microbiology Vol. 44, No. 1 P. 5-11

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Dintzis, F.R., Babcock, G.E., and Tobin, R. (1970). Studies on dilute solutions and dispersions of the polysaccharide from Xanthomonas campestris NRRL B-1459. Carbohydrate Res. 13: 257-267.

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Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Rocks. (1971). Xanthan Gum. Food Technol. 25: 22-31.

B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Tier 2 Assessments

Qualitative Tier 2 Assessment

2-Mercaptoethanol

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

2-Mercaptoethanol (2-ME) is a component in a water treatment product used to provide corrosion resistance from microbial influenced corrosion in the steel flowlines and spinelines in the produced water management collection system. Process and usage information for this chemical is summarised in **Table 1**.

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Percent Weight (%) in Product[1]
2-Mercaptoethanol	60-24-2	Biocide	1

[1] Mid-point of range provided in SDS.
CAS No = Chemical Abstracts Service Number

The product which contains 2-mercaptoethanol could potentially be used for biocide treatment in FAPA but is currently not being used. Based on its use in other Santos project areas, dosage rates in water for this chemical in the biocide are in the range of 2.1×10^{-5} mg/L.

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no carcinogenicity studies on 2-ME, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
2-Mercaptoethanol (60-24-2)	OECD 422	Liver, heart, reproductive effects	15	300	0.05	0.18

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** and the dossier regarding the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
2-Mercaptoethanol (60-24-2)	Chronic *Daphnia*	0.063	50	0.0013

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
2-Mercaptoethanol (60-24-2)	[a]	-	-	0.00085

[a]Calculated using equilibrium partitioning method.
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
2-Mercaptoethanol (60-24-2)	[a]	-	-	0.00003

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

The molecular structure of 2-ME is presented in **Figure 1**.

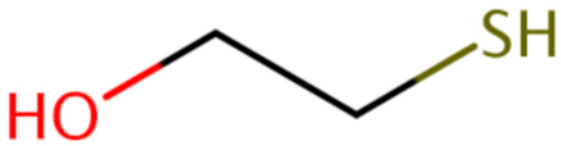

Figure 1 Molecular Structure of 2-Mercaptoethanol [2]

After evaporation or exposure to the air, 2-ME will be rapidly degraded by photochemical processes with OH-radicals. Due to the structural properties, hydrolysis is not expected to be an important fate path. Likewise, due to the soil organic carbon partition coefficient (Koc), significant adsorption e.g. to

[2] Source https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID4026343

solid soil phase is not expected. 2-ME is considered to be rapidly biodegradable in the environment. It is not expected to bioconcentrate or bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for 2-ME is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that 2-ME is not a PBT substance.

Human Health Hazards

2-ME is metabolised to its acetate salt and excreted via urine. 2-ME has moderate acute toxicity by the oral and inhalation routes; and, is more acutely toxic by the dermal route. It is irritating and considered a skin sensitiser.

In repeated dose exposure studies, it is not substantially toxic via the oral route of exposure. No information about repeated dermal toxicity or inhalation toxicity is available. No maternal or developmental toxicity was seen in animals exposed to 2-ME by the oral route. 2-ME is not genotoxic.

Based on a review of an OECD 422 study in male and female rats, TRVs were derived for 2-ME. The drinking water guideline value derived for 2-ME using the non-carcinogenic oral RfD is 0.18 mg/L (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Based on its potential use as a biocide in produced water flow lines, 2-ME may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to 2-ME in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay), and treatment and retention (and associated biodecay) are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of the biocide in produced water would be diluted by a factor of at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, 2-ME is overall moderately toxic to aquatic organisms. Acute toxicity towards algae and aquatic invertebrates is of the same order of magnitude. However, *Daphnia magna* was more sensitive (ECHA).

2-ME is readily biodegradable and does not persist in the environment. It is not expected to bioconcentrate or bioaccumulate nor is it expected to pose a substantial toxic concern to environmental receptors.

PNECs for 2-ME are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs in water. There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, estimated Water Management Facility (WMF) pond influent concentrations (1.4×10^{-10} mg/L, refer **Attachment 2**) are well less than PNECs for aquatic receptors (1.3×10^{-3} mg/L). Blending within the storage pond, degradation during storage and treatment would further reduce concentrations.

References

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Australian Environmental Agency (AEA). (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia. Available: http://www.nepc.gov.au/resource/chemical-risk-assessment-guidance-manuals

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.

Attachment 1 Risk Assessment Dossier

2-MERCAPTOETHANOL

This dossier on 2-mercaptoethanol (2-ME) presents the most critical studies pertinent to the risk assessment of its use in drilling muds, hydraulic fracturing fluids and water treatment systems. No sufficient data exist for this particular substance. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from The National Industrial Chemicals Notification and Assessment Scheme (NICNAS, 1994) and the ECHA database that provides information on chemicals that have been registered under the European Union (EU) REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – 2-Mercaptoethanol was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. 2-Mercaptoethanol was assessed as a tier 1 chemical for acute toxicity of fish and algae, a tier 3 chemical for acute toxicity of invertebrates based on a limited single acute toxicity study and a tier 2 chemical for chronic toxicity. Based on its potential for rapid degradation in the environment, it is not expected to pose a substantial toxic concern to environmental receptors. Therefore, 2-mercaptoethanol is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

2-ME is expected to rapidly degrade in the environment. It is not expected to bioconcentrate or bioaccumulate. 2-ME is metabolised to its acetate salt and excreted via urine. It is irritating and considered a sensitiser. 2-ME is not genotoxic nor is it substantially toxic via the oral route of exposure. Overall, 2-ME is moderately toxic to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-sulfanylethanol
CAS RN: 60-24-2
Molecular formula: C_2H_6OS
Molecular weight: 78.14 g/mol

Synonyms: 2-mercaptoethanol, Mercaptoethanol, Beta-Mercaptoethanol, Thioglycol, Ethanol, 2-mercapto-,2-Sulfanylethanol

3 PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of Physico-Chemical Properties of 2-ME

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	Water-white liquid	1	ECHA
Melting Point	-100°C @ 101.3 kPa	1	ECHA
Boiling Point	155.8°C @ 101.3 kPa	1	ECHA
Density	1100 kg/m^3 @ 20°C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour Pressure	130 Pa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	-0.056 @ 25°C	1	ECHA
Water Solubility	1,000 g/L @ 20°C	1	ECHA
Dissociation Constant (pKa)	9.72 @ 25°C	1	ECHA
Viscosity	3.22 mPa s @ 20°C	1	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for 2-ME.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

2-ME is expected to degrade in the environment. It has a low potential for adsorption to soil or sediment and is not expected to bioconcentrate or bioaccumulate.

B. Partitioning

2-ME is highly soluble in water. Volatilization from moist soil surfaces or water is not expected to be an important fate process based upon an estimated Henry's Law constant of $1.8X10^{-2}$ Pa-m^3/mole. 2-ME may volatilize from dry soil surfaces based upon its vapor pressure. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions (PubChem).

C. Biodegradation

In an OECD 310 test, biodegradation was 69% after 60 days (ECHA) [Kl. score = 1]. In an OECD 301A test, biodegradation was <10% after 28 days (ECHA) [Kl. score = 1]. In an OECD 301C test,

biodegradation was >15% and <21% after 28 days (ECHA) [Kl. score = 2]. In an OECD 302 C test, biodegradation was 90% after 28 days (ECHA) [Kl. score = 2].

In an OECD 309 test, the mineralisation of 2-ME in surface water was determined in a GLP-compliant study following OECD guideline 309. Mineralisation was a significant route of degradation and activity recovered as carbon dioxide (CO2) increased to >60% after 14 days of incubation at two different test concentrations. Three major transformation products were detected which exceeded 10% of applied activity at both test concentrations. A transformation product reached a maximum of 26% after 4 hours (0.17 days) at the low-test concentration and a maximum of 13% after 8 hours (0.33 days) at the high test concentration, and then decreased to non-detectable amounts after 6 days of incubation (both concentrations). A transformation product reached a maximum of 36% (low test concentration) and 30% (high test concentration) after 2 days and then decreased to 14% after 9 days of incubation (low test concentration) and to <5% after 14 days of incubation (high test concentration). Another transformation product reached a maximum of 41% (low test concentration) and 39% (high test concentration) after 4 hours (0.17 days) and then decreased to non-detectable amounts after 6 days of incubation. It was concluded that 2-ME degrades quickly in water, with a half-life of 0.079 days, and no parent compound was detected in the water layers of both test concentrations after 1 day of incubation. Based on the results of the OECD 309 study, the substance degrades in the aquatic environment to a level of >70% within a 28-day period and therefore, the substance is considered to be rapidly biodegradable (ECHA) [Kl. score = 1].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

As calculated using KOCWIN v2.00, the K_{oc} of 2-ME is 1.904 (corrected log K_{oc} = 0.2798). After exposure to soil, significant adsorption to solid soil phase (e.g. clay) is not expected (ECHA) [Kl Score=2]. Based upon this K_{oc} value, if released to soil, 2-ME is expected to have very high mobility. If released into water, based on its high water solubility, it is also not expected to adsorb to suspended solids and sediment in water.

No fugacity calculations were performed as the substance has limited persistence.

E. Bioaccumulation

No bioconcentration studies have been conducted on 2-ME. 2-ME is not expected to bioaccumulate based on the measured low experimental log K_{ow} value of -0.056 at pH 7 (ECHA) [Kl. score = 2].

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

2-ME is metabolised to its acetate salt and excreted via urine. It is irritating and considered a skin sensitiser. 2-ME is not genotoxic nor is it substantially toxic via the oral route of exposure.

B. Acute Toxicity

The oral LD_{50} values in rats are 98-169 mg/kg based on sodium-2-mercaptoethanol (CAS No. 37482-11-4) (ECHA) [Kl. score = 1].

BASF reported an oral LD_{50} value of < 112 mg/kg for rabbits (study from 1967) and an oral LD_{50} value of 336 mg/kg for rats (study from 1964) (ECHA) [Kl. Scores = 2].

The 4-hour whole body inhalation LC_{50} in rats is 2000 mg/m^3. Findings indicate effects on central nervous system, respiratory and circulatory systems and possibly on the liver. (ECHA). [Kl. score 2]

The dermal LD_{50} values in rabbits are 112 - 224 mg/kg, respectively. All animals (3/3) died in the high dose group with no specific resorptive intoxication symptoms. One animal (1/3) died in the mid dose group showing apathy, local reddening and edema as clinical signs. No animal (0/3) died in the low dose group showing apathy and local inflammation. (ECHA). [Kl. score =]

C. Toxicokinetics

The chemical structure and the observed systemic effects after exposure via different application routes clearly indicate absorption and distribution after oral and dermal administration of 2-ME. In mammals, 2-ME is rapidly excreted via urine. 2-Mercaptoacetate was detected as the main metabolite in the urine of a person who died from ingesting 2-ME. The available in vitro and in vivo data suggest metabolism of 2-ME via formation of 2-mercaptoacetate through the combined effects of alcohol dehydrogenase and aldehyde dehydrogenase. The effects after repeated oral administration of 2-ME and sodium 2 -mercaptoacetate are similar at comparable doses, thus giving additional evidence of 2-mercaptoacetate formation as the main metabolic pathway of 2-ME.

D. Irritation

Application of 2-ME to the skin of rabbits for 4 hours under occlusive conditions was considered irritating (ECHA) [Kl. score = 2]. Instillation of 2-ME into the eyes of rabbits was corrosive when the eyes were not rinsed and irritating when the eyes were rinsed (ECHA) [Kl. scores = 2].

E. Sensitisation

2-ME was considered a skin sensitiser when tested in a guinea pig maximisation test (ECHA) [Kl. score = 2].

F. Repeated Dose Toxicity

2-ME was tested in a combined repeated dose toxicity study with a reproduction/developmental toxicity screening (OECD TG 407 and 422) test. Male and female Sprague Dawley (SD) rats were dosed by oral gavage with 0, 15, 50, or 75 milligrams per kilogram (mg/kg) 2-ME over a study period of about 7 weeks. No toxic effects were recorded in the 15 mg/kg animals. A slightly higher body weight gain and food consumption was seen in the >50 mg/kg females (not significant, also at higher dose levels), whereas the >50 mg/kg males showed a significant lower body weight gain (-11 to -24%) compared to controls. Ptyalism was observed in both genders at >50 mg/kg. The >50 mg/kg males showed paleness and accentuated lobular pattern of the liver at necropsy, and minimal to marked vacuolated hepatocytes was seen in the histopathologic examination accompanied by lower blood cholesterol and triglyceride. The 75 mg/kg males had significantly increased absolute and relative liver weight (22 and 36%, respectively) and minimal to slight hypertrophy of hepatocytes. In the >50 mg/kg females, absolute and relative liver weight were significantly increased, and paleness of the liver was detected at termination; histopathological examinations showed minimal to slight liver cell hypertrophy, and increased incidence and severity of vacuolated hepatocytes. The incidence and severity of cardiomyopathy was increased in the 75 mg/kg males and in the >50

mg/kg females. There were no effects seen in the hematology, seminology and urine analysis. The no observed adverse effect level (NOAEL) is 15 mg/kg-day (ECHA) [Kl. score = 1].

G. Genotoxicity

In Vitro Studies

The *in vitro* genotoxicity studies on 2-ME are presented in **Table 3.**

Table 3 *In vitro* Genotoxicity Studies on 2-ME

Test System	Results		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains	-	-	2	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	2	ECHA
Chromosomal aberrations (human lymphocytes)	-	-	2	ECHA

*+, positive; -, negative

In Vivo Studies

Male and female mice were given a single intraperitoneal injection of 0, 50, 100 or 300 mg/kg 2-ME. The 300 mg/kg dose resulted in clinical signs of toxicity. The >100 mg/kg males had a decrease in the ratio of polychromatic to normochromatic erythrocytes, indicating bone marrow toxicity. The 300 mg/kg males showed a slight, but statistically significant, increase in the frequency of micronucleated polychromatic erythrocytes (MPE), but data generated in the additional analysis (further 2,000 polychromatic erythrocytes per animal evaluated) showed no significant difference between the 300 mg/kg males and the controls. There were no other increases in MPE in the other treated groups. Thus, it was concluded that 2-ME was not genotoxic in this study (ECHA) [Kl. score = 1].

H. Carcinogenicity

No studies are available.

I. Reproductive Toxicity/Developmental Toxicity

2-ME was tested in a combined repeated dose toxicity study with a reproduction/developmental toxicity screening (i.e., OECD TG 422) test. Male and female SD rats were dosed by oral gavage with 0, 15, 50 or 75 mg/kg 2-ME. Males were treated 5 weeks before mating, during mating and post-mating period until sacrifice after approximately 7 weeks. Females were treated 5 weeks before mating, during mating and pregnancy and lactation until day 21 post-partum inclusive except at the mid and high dose when treatment was interrupted from days 19 and 20 post coitum (PC) until delivery due to toxic effects (see below); all females were sacrificed on day 21 post-partum. There were no treatment-related effects on mating and fertility parameters at any dose level. Seminology in males revealed no effects on sperm count, motility and morphology. The estrous cycle, mating

and fertility indices, and pre-coital time were not affected, and no treatment-related effects were detected in reproductive organs on macro- or microscopic examination. Maternal toxicity was evident with deaths of pregnant females at >50 mg/kg (six dead or sacrificed on PC days 19-23 at 75 mg/kg, three dead on PC day 21 or day 2 post-partum at 50 mg/kg). Surviving females in the mid- and high-dose groups showed higher body weight gain (>52 %) and food consumption (14%; statistically significant in the high-dose group) during the pre-mating period and lactation, while those in the top-dose group had reduced body weight gain (-47% in last week of pregnancy). Effects on body weight gain and food consumption were considered by the investigators to be treatment related.

At 75 mg/kg, the duration of gestation was increased (22.3 days v 21.5 days in controls) and the number of live born pups/litter was significantly decreased due to one dam with only one live born pup. The number of females with live-born pups was reduced in the mid- and high-dose groups (7/10 and 4/10 versus 8/9 in controls; statistically significant at the high dose). Gestation indices were given as 78% and 40% in the mid- and high-dose groups compared to 100% in the low-dose group and the controls. There was no effect on sex ratio.

The primary treatment-related effect on reproduction in the TG 422 study was prolonged labour and dystocia at dose levels of >50 mg/kg. Certain aliphatic thiol compounds, including 2-ME, have been shown to act as antagonists to the neuropeptide oxytocin, blocking the contractile response of oxytocin on the rat uterus in vitro (Martin and Schild, 1965). Oxytocin is secreted primarily by the posterior pituitary gland and is critical to the normal progress of parturition and sustaining sufficient uterine contractions during labour to expel the foetus(es) and to ligate severed blood vessels within the contracted myometrium after the placenta separates, thus preventing haemorrhage. It is possible that oral administration of 2-ME to pregnant rats in the TG 422 study was sufficient to disrupt the normal oxytocin-mediated progression of parturition by diminishing uterine contractions and prolonging labour.

Slightly higher pup body weights were noted at birth in the 75 mg/kg group, probably as a result of the slight increase in the length of pregnancy. However, despite these higher pup weights at birth, mean pup body weight at 75 mg/kg was lower than control values throughout the remainder of the lactation period as a result of significantly lower pup body weight gain beginning on postnatal day 4. It is not clear whether the effects on pup body weight and survival at 75 mg/kg are the result of direct exposure to the test article in utero or via the milk or perhaps secondary to maternal care issues related to the condition of the dams or an effect on maternal milk production. Oxytocin is known to play an important role, not only in parturition, but also in milk production during lactation. Given the potential antagonistic effects of 2-ME on oxytocin, it is possible that maternal exposure to 2-ME during lactation may hinder milk production and consequently pup growth and viability.

In addition to the effects on parturition and pup body weight, mean live litter size was significantly ($p<0.5$) lower in the 75 mg/kg group compared to the control group (10.0 versus 14.9 pups). The smaller litter size at 75 mg/kg was primarily attributed to one dam (out of 4 surviving dams) that delivered a single pup. This reduction in mean live litter size correlated with higher post-implantation loss and decreased pup survival at the same dose level. However, the small number of surviving dams/litters available for evaluation at 75 mg/kg (n=3 or 4 dams) is a potential major confounding factor in establishing a relationship between these endpoints (live litter size and pup survival) and test article administration. No apparent effects on mating or fertility indices or on male reproductive parameters were observed at any dose level evaluated. The NOAELs for reproductive toxicity are 75 and 15 mg/kg-day for males and females, respectively. The NOAEL for parental

systemic toxicity is 15 mg/kg-day. The NOAEL for developmental toxicity is 15 mg/kg-day (ECHA) [Kl. score = 1].

A reproductive/developmental toxicity screening (OECD TG 421) study was conducted on sodium mercaptoacetate. 2-ME is metabolised in the body to 2-mercaptoacetate. Male and female SD rats were dosed by oral gavage with 0, 20, 40 or 80 mg/kg sodium mercaptoacetate (0, 16, 32 or 64 mg/kg mercaptoacetic acid). In the 80 mg/kg group, there were two males and one female that were found dead during the pre-mating or mating periods with no clinical signs observed before death and no relevant post-mortem findings. On gestation day (GD) 23 PC, 3/11 surviving 80 mg/kg females were found dead, all having delivered pups, although one female had one foetus in the vagina and still had 11 dead foetuses in the uterine horns at necropsy. Another pregnant female with dead and live foetuses in the uterine horns was sacrificed on GD 23 because of poor clinical condition. One additional 80 mg/kg female was prematurely sacrificed on lactation day (LD) 1 because all the pups were dead, and another female was found dead on LD 2. One 40 mg/kg female was found dead on GD 22, pregnant with dead foetuses in the uterine horns. Ptyalism [excess saliva] was observed in the > 40 mg/kg animals and may have been related to the taste of the test material. Mean body weight gains and generally feed consumption were unaffected by treatment. Vaginal cyclicity was unaffected by treatment. There were no effects on male or female mating behaviour or fertility; embryo-foetal development was considered unaffected by treatment. The 80 mg/kg females had a significantly longer gestation period (22.8 vs. 21.6 days, controls). Mean pup body weight gain was significantly lower between post-natal day (PND) 1 and 5 in the >40 mg/kg groups, but there was no treatment-related clinical signs or post-mortem findings. Sperm morphology, motility and counts were unaffected by treatment. The mean liver and kidney weights were slightly but statistically significantly higher for the 80 mg/kg males. The higher liver weights correlated with a trend towards increased glycogen content at this dose level, an effect that was considered to be toxicologically important. There were no corresponding histopathological changes for the kidney weight changes. The mean absolute seminal vesicle weights were significantly lower for the >20 mg/kg males and were dose-related; this correlated with a slight decrease in secretory content in the seminal vesicles observed microscopically of the 80 mg/kg males. The NOAEL for male reproductive toxicity is 64 mg/kg-day as mercaptoacetic acid. The NOAEL for female reproductive toxicity is 16 mg/kg-day as mercaptoacetic acid, based on deaths in late gestation and delayed delivery. NOAEL for parental toxicity is 16 mg/kg-day as mercaptoacetic acid, based on mortality. The NOAEL for offspring toxicity is 32 mg/kg-day as mercaptoacetic acid based on the dead litter at 64 mg/kg-day (ECHA) [Kl. score = 1].

Pregnant female Wistar rats were dosed by oral gavage with 0, 5, 15 or 25 mg/kg 2-ME on gestational days 6 to 19. There was no maternal or developmental toxicity. The NOAEL for maternal and developmental toxicity is 25 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for 2-ME follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

An OECD 422 study was conducted on 2-ME. Males were treated 5 weeks before mating, during mating and post-mating period until sacrifice after ca. 7 weeks. Females were treated 5 weeks before mating, during mating and pregnancy and lactation until day 21 post-partum inclusive except at the mid and high dose when treatment was interrupted from days 19 and 20 PC until delivery due to toxic effects; all females were sacrificed on day 21 post-partum. The NOAEL for female

reproductive toxicity and parental systemic toxicity is 15 mg/kg-day. The NOAEL of 15 mg/kg-day will be used to derive the oral reference dose.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 15/(10 x 10 x 1 x 3 x 1) = 15/300 = 0.05 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)
Drinking water guidance value = (0.05 x 70 x 0.1)/2 = 0.18 mg/L

K. Human Health Hazard Assessment Of Physico-Chemical Properties

2-ME does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Overall, 2-ME is moderately toxic to aquatic organisms as noted below.

B. Aquatic Toxicity

Table 4 lists the results of acute aquatic toxicity studies on salts of 2-ME.

Table 4 Acute Aquatic Toxicity Studies on Salts of 2-ME

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Leuciscus idus	96-hr LC_{50}	37	2	ECHA
Daphnia magna	48-hr EC_{50}	0.4	2	ECHA
Desmodesmus subspicatus	96-hr EC_{50} NOEC	19 1.7	1	ECHA

The 21-day no observed effect concentration (NOEC) from a *Daphnia* reproduction test was determined to be >0.063 mg/L with a lowest observed effect concentration (LOEC) of 0.1264 mg/l (ECHA) [Kl. score = 1]. No other chronic toxicity studies were available.

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The predicted no effect concentration (PNEC) calculations for 2-ME follow the methodology discussed in DEWHA (2009).

$PNEC_{water}$: Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (37 mg/L), *Daphnia* (0.4 mg/L) and algae (19 mg/L). Results from chronic toxicity studies are available for invertebrates (>0.063 mg/L) and algae (1.7 mg/L). On the basis that the data consists of short-term results from three trophic levels and long-term results from two trophic levels, an assessment factor of 50 has been applied to the lowest reported NOEC value of 0.063 mg/L for *Daphnia*. The $PNEC_{water}$ is 0.0013 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Moreover, the substance is not expected to substantially partition to sediments. Nonetheless, a $PNEC_{sed}$ was calculated using the equilibrium partitioning using the experimental data for K_{ow} provided in **Table 1**. The $PNEC_{sed}$ is 0.00085 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 0.836/1280 \times 1000 \times 0.0013$
$= 8.5 \times 10^{-4}$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = 0.0013 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 0.076/1000 \times 2400]$
$= 0.836\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 1.94 \times 0.04$
$= 0.076$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} was calculated via the MCI method to be 10 L/kg.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no EC_{10} or NOEC values for terrestrial receptors. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.00003 mg/kg soil dry weight.
The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (0.038/1500) \times 1000 \times 0.0013$
$= 3 \times 10^{-5}$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = 0.0013 mg/L

And:
$Kp_{soil} = K_{oc} \times f_{oc}$
$= 1.904 \times 0.02$
$= 0.038\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} was calculated via the MCI method to be 10 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

2-ME is readily biodegradable in the aquatic environment; thus, it does not meet the screening criteria for persistence.

No bioconcentration studies are available for 2-ME. The measured log K_{ow} for 2-ME is -0.056; thus, 2-ME does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on 2-ME show a NOEC of <0.1 mg/L. Thus, 2-ME meets the criteria for toxicity.

The overall conclusion is that 2-ME is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for 2-ME.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
2-Mercaptoethanol	60-24-2	Not a PBT	No	No	No	No	No	Yes	1 (fish and algae), 3 (invert)	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre

GD	gestation day
GLP	Good Laboratory Practices
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model kPa kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lactation day
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mPa · s	millipascal second
MPE	micronucleated polychromatic erythrocyte
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
Pa m³/mol	Pa cubic meter per mol
PBT	Persistent, Bioaccumulative and Toxic
PC	post coitum
PND	post-natal day
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

RfD	reference dose
SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
USEPA	United States Environmental Protection Agency

Attachment 2 Contingency Biocide Dosing Assumptions

Attachment 2
Summary of Exposure Point Concentration Development
(Contingency Water Treatment Chemicals)

Mass Balance

In other Santos project areas, approximately 413 milligrams per litre (mg/L) of a water treatment product is being dosed (9.2 litres [L] of the product added to approximately 1,380 billion barrels [bbl] or 2.2 x 10^5 litres of legacy/CF1 PFW). The constituent of potential concern (COPC) legacy/CF1 produced formation water (PFW) concentrations are calculated based on the product dose that is apportioned between the COPCs based on the COPC percent weight in the product (composition information in the safety data sheet). The concentration of the COPCs in the water storage pond influent (representative of treatment of combined produced water from legacy/CF1 PFW and bore water) was based on the combined dilution from 2,300 bbl/day.

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	COPC Legacy/CF1 PFW (mg/L)	Storage Pond Influent (mg/L)
2-Mercaptoethanol	60-24-2	1	2.1E-05	1.4E-10

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
mg/L = milligrams per litre
PFW = produced formation water

Qualitative Tier 2 Assessment

Alkanes, C11-15-iso-

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Alkanes, C11-C15-iso is a chemical in a product used in drilling and completion activities, including workovers. The workover process is designed to remove any solids from the well and facilitate placement of the pump. As part of this process, fluids and some coal fines are removed from the well and transported to produced water ponds for management within the produced water stream. Once the well has been placed and commissioned, produced water is discharged into the water gathering pipelines and conveyed to the water ponds/water treatment facilities, such as ROP2, for treatment and beneficial use (such as dust suppression, construction, operational use and stock water for cattle).

The purpose and maximum quantity for this chemical is summarised in **Table 1**.

Table 1 Initial and Underbalance Workover Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Alkanes, C11-15-iso-	90622-58-5	Activators, Emulsifiers and Neutralisers	NA

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number
NA = quantity used varies

No data on alkanes, C11-15-iso- were located. Data for this dossier has been read-across from similar hydrocarbon substances and from the C9-C14 aliphatic (≤2% aromatics) hydrocarbons solvents category used for the European Union Registration, Evaluation, Authorisation and Restriction of Chemicals (EU REACH). The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

C9-C14 aliphatic (≤2% aromatics) and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in **Attachment 1**. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Alkanes, C11-15-iso- (90622-58-5)	Reproductive/ Developmental Study	None	1000	300	3.33	12

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Alkanes, C11-15-iso- (90622-58-5)	-	-	-	0.001[a]

[a] PNEC estimated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Alkanes, C11-15-iso- (90622-58-5)	[a]	-	-	260

[a] PNEC estimated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Alkanes, C11-15-iso- (90622-58-5)	[a]	-	-	100

[a] PNEC estimated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

The C11-C15 iso alkanes are comprised of complex aliphatic hydrocarbon solvents that contain >98% aliphatic constituents with carbon numbers in the range of C11-C15 and less than 2% aromatic constituents. The chemical constituents in this complex Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB) substance may include straight chain (n-), branched (iso-) and cyclic aliphatic hydrocarbons but have less than 2% aromatic hydrocarbons. The molecular structure of alkanes, C11-15-iso is presented in **Figure 1**.

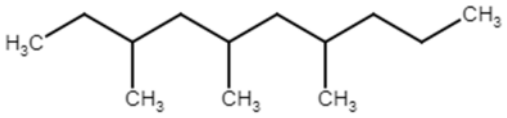

Figure 1 Molecular Structure of Alkanes, C11-15-iso[2]

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/90622-58-5

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. The alkanes, C11-15-iso- are expected to highly absorb to sediment and soil. Alkanes, C11-15- iso- is expected to have constituents with the potential to bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for alkanes, C11-15-iso is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that alkanes, C11-15-iso is not a PBT substance.

Human Health Hazards

The acute toxicity of C9-C14 aliphatic hydrocarbons (≤2% aromatics), which includes the alkanes, C11-15-iso-, is low by the oral, dermal and inhalation route. It is, however, an aspiration hazard. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not skin or eye irritants or a dermal sensitiser.

Repeated inhalation exposure of rats to a C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluid showed no target organ effects; oral exposures to very high doses of these hydrocarbons showed irritation to the gastrointestinal tract and effects in the liver that likely represent an adaptive response to the metabolism of the hydrocarbons and not a toxic response. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not genotoxic; nor do they exhibit any evidence of reproductive or developmental toxicity in rats.

A reproductive/developmental toxicity study was conducted on a C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid in rats. There were no adverse effects at 1,000 milligrams per kilogram-day (mg/kg-day), the highest dose tested. The no observed adverse effect level (NOAEL) of 1,000 mg/kg-day was used to derive the oral RfD and the drinking water guideline value (12 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Following water treatment, alkanes, C11-15-iso may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to alkanes, C11-15-iso in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, overall, alkanes, C11-15-iso- are expected to ultimately biodegrade in the environment.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km

downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

Based on an evaluation of aquatic toxicity tests in similar hydrocarbons, alkanes, C11-15-iso- has a low acute toxicity concern to aquatic life. Acute toxicity towards aquatic invertebrates and algae is of the same order of magnitude. However, fish were more sensitive in chronic toxicity testing (ECHA).

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. BCF values calculated for representative hydrocarbon structures in the group do not indicate a potential for bioaccumulation (BCF values <2,000).

PNECs for alkanes, C11-15-iso are provided in **Tables 3 – 5**. As noted in the tables, there are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the quantitative structure activity relationship (QSAR) model PETRORISK v7.04. The QSAR model was also used to calculate a PNEC for water. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, estimated Water Management Facility (WMF) pond influent concentrations (2.2×10^{-7} mg/L, refer **Attachment 2**) are well less than PNECs for aquatic receptors (1×10^{-1} mg/L). Blending within the storage pond, degradation during storage and treatment would further reduce concentrations.

References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019.

Australian Environmental Agency (AEA). (2009). Environmental Risk Assessment Guidance Manual for Industrial Chemicals, Commonwealth of Australia. Available: http://www.nepc.gov.au/resource/chemical-risk-assessment-guidance-manuals

Department of the Environment and Energy (DoEE). (2017). Exposure draft: Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction. Commonwealth of Australia, available at http://www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.

Santos, 2013. Dawson River Release Scheme – Environmental Authority Amendment Application – Supporting Information. May 2013.

Attachment 1 Risk Assessment Dossier

ALKANES, C11-15-ISO-

This dossier on alkanes, C11-15-iso- presents the most critical studies pertinent to the risk assessment of alkanes, C11-15-iso- in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Alkanes, C11-15-iso- was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Alkanes, C11-15-iso- was assessed as a tier 2 chemical for chronic toxicity. Therefore, alkanes, C11-15-iso- is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

The C11-C15-iso- alkanes are comprised of complex aliphatic hydrocarbon solvents that contain >98% aliphatic constituents with carbon numbers in the range of C11-C15 and less than 2% aromatic constituents. The chemical constituents in this complex UVCB substance may include straight chain (n-), branched (iso-) and cyclic aliphatic hydrocarbons but have less than 2% aromatic hydrocarbons.

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. Members of this group are insoluble and are expected to highly adsorb to sediment and soil. Based on similar substance, C11-C15-iso- alkanes are not expected to bioaccumulate and have a low acute toxicity concern to aquatic life.

The acute toxicity of similar substance C9-C14 aliphatic hydrocarbons (≤2% aromatics), which includes the alkanes, C11-15-iso-, is low by the oral, dermal and inhalation route. It is, however, an aspiration hazard. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not skin or eye irritants or a dermal sensitiser. Repeated inhalation exposure of rats to a C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluid showed no target organ effects; oral exposures to very high doses of these hydrocarbons showed irritation to the gastrointestinal tract and effects in the liver that likely represent an adaptive response to the metabolism of the hydrocarbons and not a toxic response. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not genotoxic; nor do they exhibit any evidence of reproductive or developmental toxicity in rats.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Alkanes, C11-15-iso-
CAS RN: 90622-58-5
Molecular formula: Not available (UVCB substance)
Molecular weight: Not available (UVCB substance)
Synonyms: Alkanes, C11-15-iso-; C11-15 isoalkanes

3 PHYSICO-CHEMICAL PROPERTIES

Physical and chemical properties were not available for the UVCB hydrocarbon. As a result, information was obtained from a read-across substance (alkanes, C12-14-iso-). Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Alkanes, C12-14-iso- (CAS No. 68551-19-9)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid with a faint odour	2	ECHA
Melting point	-114°C @ 101.3 kPa (pour point)	2	ECHA
Boiling point	189 to 206°C @ 101.3 kPa	2	ECHA
Density	760 kg/m^3 @ 15°C	2	ECHA
Vapour pressure	40 Pa @ 20°C	2	ECHA
Partition coefficient (log K_{ow})	5.94 to 7.14 (pH and temperature not calculated)	-	ECHA
Water solubility	0.00001 to 0.00015 g/L	-	ECHA
Viscosity	1.77 mm^2/s @ 20°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No other specific environmental regulatory controls or concerns were identified within Australia and internationally for alkanes, C11-15-iso-.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Aliphatic hydrocarbons composed of branched (isoalkanes) and cyclic aliphatic hydrocarbons in the C10 to C16 range have reported to be readily biodegradable to not inherently biodegradable. The alkanes, C11-15-iso- are insoluble and are expected to highly adsorb to sediment and soil. They are not expected to bioaccumulate.

B. Partitioning

Based on Henry's Law Constant values > 4.76 x 10^4 Pa-m^3/mol @25 °C, members of this group have the potential to volatilize from water or moist soil surfaces. These chemicals are unlikely to degrade by hydrolysis as they lack a functional group that is hydrolytically reactive. However, in the air, category members have the potential to rapidly degrade through indirect photolytic processes (OECD, 2012).

C. Biodegradation

In an OECD 301F test, hydrocarbons, C10-C13, isoalkanes, cyclics (<2% aromatics) degraded 89.8% after 28 days, indicating ready biodegradation (ECHA) [Kl. score = 2].

In an OECD 301F test, hydrocarbons C12-16, isoalkanes, cyclics (<2% aromatics) degraded 22% after 28 days and 50% after 70 days, indicating inherent biodegradation (ECHA) [Kl. score 2].

In a USEPA OTS 796.3100 aerobic aquatic biodegradation test, hydrocarbons, C13-C15, isoalkanes, cyclics (<2% aromatics) degraded 16.95% after 24 days and 20.62% after 31 days, indicating that it is not inherently but ultimately biodegradable (ECHA) [Kl. score = 2].

In a USEPA OTS 796.3100 aerobic aquatic biodegradation test, hydrocarbons, C12-C13, isoalkanes, cyclics (<2% aromatics) degraded 12.69% after 24 days and 13.69% after 31 days, indicating that it is not inherently but ultimately biodegradable (ECHA) [Kl. score = 2].

Overall, alkanes, C11-15-iso- are expected to ultimately biodegrade in the environment. If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

Alkanes, C11-15-iso- is a UVCB substance. The standard tests to determine the K_{oc} are for single substances and not for UVCB substances. Therefore, a K_{oc} value for C11-15-iso- was not determined.

The calculated K_{oc} values for linear aliphatic hydrocarbons dodecane and tetradecane are 110,000 and 759,000 L/kg, respectively, using SPARC v4.2 program in the CONCAWE Library of PETRORISK (ECHA). This modelled range of K_{oc} values are consistent with those presented in the review of C10 – C12 aliphatics by TPHCWG (1997). These values, along with the low solubility of substances in this group, suggest that alkanes, C11-15-iso- will highly adsorb to sediment and soil.

E. Bioaccumulation

Alkanes, C11-15-iso- is a UVCB substance. The calculated BCF values for linear aliphatic compounds undecane (C11), dodecane (C12), and tetradecane (C14) are 337.8, 790.9, and 962.9 L/kg, respectively, using the BCFWIN V2.16 model within EPISuite 3.12. The predicted BCFs for hydrocarbons are considered to be generally overly conservative because biotransformation is not quantitatively taken into account. For these linear aliphatic hydrocarbons, based on BCFs for indicator compounds - the values indicate that they are not expected to bioaccumulate.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of C9-C14 aliphatic hydrocarbons (≤2% aromatics), which includes the alkanes, C11-15-iso-, is low by the oral, dermal and inhalation route. It is, however, an aspiration hazard. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not skin or eye irritants or a dermal sensitiser. Repeated inhalation exposure of rats to a C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluid showed no target organ effects; oral exposures to very high doses of these hydrocarbons showed irritation to the gastrointestinal tract and effects in the liver that likely represent an adaptive response to the metabolism of the hydrocarbons and not a toxic response. C9-C14 aliphatic hydrocarbons (≤2% aromatics) are not genotoxic; nor do they exhibit and evidence of reproductive or developmental toxicity in rats.

B. Acute Toxicity

The oral LD_{50} in rats for C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids is >5,000 mg/kg (ECHA) [Kl. score = 2].

The 4-hour inhalation LC_{50} in rats for C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids is > 4,951 mg/m^3 [ECHA) [Kl. scores =1 and 2].

The dermal LD_{50} in rats for C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids is >5,000 mg/kg (ECHA) [Kl. score = 2].

C. Irritation

The C9-C14 aliphatic, ≤2% aromatic hydrocarbon fluids are neither skin nor eye irritants (ECHA) [Kl. scores = 1 and 2].

D. Sensitisation

C9-C14 aliphatic, <2% aromatic hydrocarbon fluids were not skin sensitisers when tested in guinea pig maximisation tests (ECHA) [Kl. score = 2].

A C9-C14 aliphatic, <2% aromatic hydrocarbon fluid showed no indication of skin sensitisation in a human repeated insult patch test (ECHA).

E. Repeated Dose Toxicity

Oral

Male and female rats were dosed by oral gavage with 0, 500, 2,500 or 5,000 mg/kg with a C9- C14 aliphatic (<2% aromatic) hydrocarbon fluid 7 days/week for 13 weeks. Additional groups of animals were dosed with 0 or 5,000 mg/kg for 13 weeks, followed by a 4-week recovery period. There were dose-related changes in the hematology and serum chemistry parameters which were consistent with changes seen in the liver. Hepatocellular hypertrophy (liver cell enlargement) were seen in both males and females in all dose groups and were reversible. The liver effects were not considered to be an indication of toxicity but an adaptive response due to the metabolism of the hydrocarbons. There were also mucosal thickening and other signs of irritation to the stomach and anus, which appeared to be the direct result of high-dose intubation of a locally irritating material. All treatment-related effects were reversible within the 4-week recovery period. The NOAEL for systemic effects in this study is considered to be 5,000 mg/kg-day (ECHA) [Kl. score = 1].

Hydrocarbons C11-C14, n-alkanes, isoalkanes, cyclics (<2% aromatics) (CAS RN 64742-47-8). Tested in a 90 day repeated oral toxicity test (OECD TG 408) in Sprague Dawley rats. The study design included a 28 day recovery period for rats exposed to the highest dose (1000 mg/kg/day). The NOAEL was 1000 mg/kg/day (OECD 2012) [Kl Score = 2].

Hydrocarbons C10-C12 isoalkanes (<2% aromatics) (CAS RN 64742-47-8). Tested in a 90 day repeated oral toxicity test (OECD TG 408) in Sprague-Dawley rats. The study design included a 28 day recovery period for rats exposed to the highest dose (1000 mg/kg/day). The NOAEL was 1000 mg/kg/day (OECD 2012) [Kl Score = 2].

Inhalation

Male and female rats were exposed by inhalation to 0, 2,600, 5,200, or 10,400 mg/m^3 of a C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid, 6 hours/day, 5 days/week for 13 weeks. There were no mortality or effects in either the hematology or the serum chemistry parameters. The male rats at all dose levels had increased liver and kidney weights; male heart weights were also increased at 10,400 mg/m^3 and kidney weights were increased in the 10,400 mg/m^3 group. Kidney effects indicative of alpha-2u-globulin nephropathy were observed at all dose levels. There were no other effects that were considered to be treatment-related. The alpha-2u-nephropathy in the male rats are not considered to be relevant to humans; for the organ weight changes other than the male kidneys, there were no corresponding histopathologic changes. The NOAEL for this study is 10,400 mg/m^3, the highest exposure concentration tested (ECHA) [Kl. score = 1].

Dermal

No studies are available.

F. Genotoxicity

In Vitro Studies

The key *in vitro* genotoxicity studies on C9-C14 aliphatic hydrocarbons (≤2% aromatics) are presented in Table 3.

Table 3 In vitro Genotoxicity Studies on C9-C14 Aliphatic Hydrocarbons (≤2% Aromatics)

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* and *E. coli* strains)	-	-	1	ECHA
Mammalian cell gene mutation (Chinese hamster V 79 cells)	-	-	2	ECHA
Chromosomal aberration (human lymphocytes)	-	-	1	ECHA

*+, positive; -, negative

In Vivo Studies

In two separate studies involving two different C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids, male and female CD-1 mice were given a single oral gavage dose at concentrations of 0, 1,250, 2,500, or 5,000 mg/kg. The frequency of micronucleated polychromatic erythrocytes was not significantly increased in the treated mice compared to that in the controls (ECHA) [Kl. Score = 1].

In two separate dominant lethal studies involving two different C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids, male rats were exposed 6 hours/day for 5 consecutive days to exposure concentrations of 0, 300, or 900 ppm. There was no evidence of a mutagenic response in the treated rats (ECHA) [Kl. score = 2].

G. Carcinogenicity

No carcinogenicity studies are available on the C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids.

H. Reproductive Toxicity

A C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid was tested in a combined repeated dose toxicity study with a reproductive/developmental toxicity screening test (OECD 422). Male and female SD rats were given oral gavage doses of 0, 25, 150, or 1,000 mg/kg-day. There was no indication of reproductive toxicity at any dose level. The NOAEL for reproductive toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

A C9-C14 aliphatic, <2% aromatic hydrocarbon fluid was tested in a reproductive/developmental toxicity screening test (OECD 421). Male and female SD rats were given oral gavage doses of 0, 100, 300, or 1,000 mg/kg-day. There was no indication of reproductive toxicity or any effects on the endocrine system at any dose level. The NOAEL for reproductive toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

I. Developmental Toxicity

A C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid was tested in a rat pre-natal developmental toxicity study. Pregnant female rats were exposed by inhalation to 0, 300 or 900 ppm for 6

hours/day during gestation days 6 to 15. There was no evidence of maternal or developmental toxicity at either exposure level. The NOAEL for this study is 900 ppm (ECHA) [Kl. score = 1].

Another C9-C14 aliphatic, <2% aromatic hydrocarbon fluid was tested in a rat pre-natal developmental toxicity study. Pregnant female rats were exposed by inhalation to 0, 300 or 900 ppm for 6 hours/day during gestation days 6 to 15. There was no evidence of maternal or developmental toxicity at either exposure level. The NOAEL for this study is 900 ppm (ECHA) [Kl. score = 1].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for alkanes, C11-15-iso- follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

A 13-week oral gavage study was conducted on a C9-C14 aliphatic (<2% aromatic) hydrocarbon fluid in rats. There were no adverse effects at 5,000 mg/kg-day, the highest dose tested. Alternatively, two other tests indicate that the NOAEL for this substance is 1,000 mg/kg/day. Therefore, the NOAEL of 1,000 mg/kg-day will be used to derive the oral reference dose and the drinking water guidance value for alkanes, C11-15-iso-.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 5,000/(10 x 10 x 1 x 3 x 1) = 1,000/300 = 3.33 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)

Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (3.33 x 70 x 0.1)/2 = 11.6 mg/L

Cancer

No carcinogenicity studies are available on C9-C14 aliphatic (<2% aromatic) hydrocarbon fluids. Thus, a cancer reference value was not derived for alkanes, C11-15-iso-.

K. Human Health Hazard Assessment Of Physico-Chemical Properties

Alkanes, C11-15-iso- do not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL HAZARD ASSESSMENT

A. Summary

Alkanes, C11-15-iso- has a low acute toxicity concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on hydrocarbons, C10-C12, isoalkanes (<2% aromatics).

Table 4 Acute Aquatic Toxicity Studies on C10-C12 Isoalkanes (<2% Aromatics)*

Test Substance	Test Species	Endpoint	Results (mg/L) [WAF]	Kl. score
Hydrocarbons, C10-C12, isoalkanes (<2% aromatics)	*Oncorhynchus mykiss*	96-hour LL_{50}	>1,000	1
Hydrocarbons, C10-C12, isoalkanes (<2% aromatics)	*Daphnia magna*	48-hour LL_{50}	>1,000	1
Hydrocarbons, C10-C12, isoalkanes (<2% aromatics)	*Pseudokirchnerella subcapitata*	72-hour LL_{50} 72-hour NOELR	>1,000 1,000	1

*All studies used the water accommodated fractions (WAFs) of the test substance.

Chronic Studies

The 28-day NOELR (No Observed Effect Loading Rate) for hydrocarbons, C11-13, isoalkanes (<2% aromatics) in freshwater fish is 0.316 mg/L based on growth. The value for NOELR was estimated by QSAR model – Petrotox. This model combines a partitioning model used to calculate the aqueous

concentration of hydrocarbon components with the Target Lipid Model used to calculate acute and chronic toxicity of non-polar narcotic chemicals. Petrotox computes toxicity based on the summation of the aqueous-phase concentrations of hydrocarbon block(s) that represent a hydrocarbon substance and membrane-water partition coefficients that describe the partitioning of the hydrocarbons between the water and organism (ECHA) [Kl. score = 2].

The 21-day NOELR for hydrocarbons, C11-13, isoalkanes (<2% aromatics) for *Daphnia* is 1 mg/L based on reproduction (ECHA) [Kl. score = 1].

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for alkanes, C11-15-iso- follow the methodology:

PNEC water

Using the QSAR model PETRORISK v7.04, the estimated $PNEC_{water}$ value for C11-15-iso- is 0.001 mg/L [Kl. score = 2].

PNEC sediment

Using the QSAR model PETRORISK, v7.04 the estimated $PNEC_{sediment}$ value for C11-15-iso- is 260 mg/kg soil wet weight (CONCAWE) [Kl. score = 2].

PNEC soil

Using the QSAR model PETRORISK v7.04, the estimated $PNEC_{sediment}$ value for C11-15-iso- is 100 mg/kg soil wet weight (CONCAWE) [Kl. score = 2].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Based on the existing studies for similar substances, alkanes, C11-15-iso- is expected to be readily biodegradable. Thus, alkanes, C11-15-iso- does not the screening criteria for persistence.

Alkanes, C11-15-iso- is a UVCB substance. BCF values calculated for representative hydrocarbon structures in the group do not indicate a potential for bioaccumulation (BCF values <2,000). Thus, alkanes, C11-15-iso- does not meet the screening criteria for bioaccumulation.

Read-across substance hydrocarbons, C10-C12, isoalkanes (<2% aromatics) did not exhibit acute toxicity to fish, invertebrates or algae with measured toxicity values > 1 mg/L. Aquatic chronic

toxicity values were > 0.1 mg/L. Thus, alkanes, C11-15-iso- does not meet the screening criteria for toxicity.

The overall conclusion is that alkanes, C11-15-iso- is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for alkanes, C11-15-iso-.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Alkanes, C11-15-iso-	90622-58-5	Not a PBT	No	No	No	No	No	No	1	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCFWIN	USEPA EPISuite model used to estimate bioconcentration factors
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EPISUITE	Estimation Programs Interface Suite
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LL	lethal level
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mm^2/s	square millimetres per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOELR	no observed effect loading rate
OECD	Organisation for Economic Co-operation and Development
OTS	Office of Toxic Substances
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
WAF	water accommodated fraction

Attachment 2 Mass Balance Calculations

Attachment 2
Summary of Exposure Point Concentration Development
(Initial and Underbalance Workover Fluid Chemicals)

Mass Balance

In other Santos project areas, approximately 1,540 mg/L of the product is being dosed (5 L of product added to 3,250 litres of water) during each well treatment. The product dose is apportioned between the constituents of potential concern (COPCs) based on the COPC percent weight in the product (composition information in the safety data sheet) for COPC dosage rate per well. The eight-well COPC flowback concentrations are calculated based on the treatment of eight wells per day, and dilution by produced water (3,250 L) during well flush. The concentration of the COPCs in the water storage pond influent was based on dilution from the combined average field and groundwater bore water productions (0.5 ML/d).

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	Dosage Rate per Well (mg/L)	8-Well Flowback (mg/L)	Storage Pond Influent (mg/L)
Alkanes, C11-15-iso-	90622-58-5	3.3	51	1.2E-01	2.2E-07

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
mg/L = milligrams per litre

Qualitative Tier 2 Assessment

Amine Oxides, Cocoalkyldimethyl

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Amine oxides, cocoalkyldimethyl is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Amine oxides, cocoalkyldimethyl	61788-90-7	Corrosion Inhibitor	0.00079%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no carcinogenicity studies on amine oxides, cocoalkyldimethyl, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline value is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Amine oxides, cocoalkyldimethyl (CAS No. 61788-90-7)	Dietary Study	Reduced body weight	42	100	0.4	1.5

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Amine oxides, cocoalkyldimethyl (CAS No. 61788-90-7)	*Selenastrum capricornutum*	0.09	10	0.009

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Amine oxides, cocoalkyldimethyl (CAS No. 61788-90-7)	[a]	-	-	0.21

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Amine oxides, cocoalkyldimethyl (CAS No. 61788-90-7)	[a]	-	-	0.18

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Amine oxides, cocoalkyldimethyl is a member of the amine oxides (AO) category. Chemicals in this category are surfactants, consisting of a polar “head” (the amine oxide) and a relatively inert, hydrophobic “tail” (the long alkyl substituent). The chemicals of the amine oxides category do not exist as ‘pure’ substances, but are produced, transported and used as aqueous solutions, typically within a range of 25-35% AO/water. The AOs are produced and used either as single chain length substances (e.g., C_{12}) or as a mixture of different chain lengths (e.g., C_{12} to C_{18}). The most common AO in commerce is the alkyl dimethyl AO, where the alkyl group contains 10 to 16 carbon atoms, predominately C_{12} and C_{14}, and the average chain length is $C_{12.9}$.

The molecular structure for a C_{12} dimethyl amine oxide, is presented in **Figure 1**.

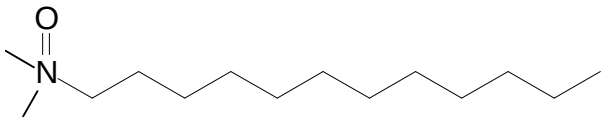

Figure 1 Molecular Structure of C_{12} dimethyl amine oxide [2]

Amine oxides, cocoalkyldimethyl is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for absorption to soil and sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for amine oxides, cocoalkyldimethyl is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

Amine oxides, cocoalkyldimethyl does not exhibit significant acute oral or dermal toxicity. It appears to be a skin and eye irritant but it is not a skin sensitiser. It is not a reproductive or developmental toxicant, genotoxic or expected to be a carcinogen. Overall, amine oxides, cocoalkyldimethyl is moderately toxic to aquatic organisms.

In a 2-year dietary study, C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) was administered to male and female rats for 104 weeks. The estimated daily intakes were: 0, 4.24, 42.3, or 87.4 mg/kg-day for males; and 0, 5.23, 52.6, or 107 mg/kg-day for females. Survival, clinical chemistry, opthalmoscopic exams, clinical signs, gross pathology, and histopathology were similar across groups. The 0.2% animals had reduced body weights of >10%. The no observed adverse effect level (NOAEL) is 42 milligrams per kilogram-day (mg/kg-day), based on reduced body weight. The NOAEL from this study was used for determining the oral RfD and the drinking water guideline value (1.5 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Amine oxides, cocoalkyldimethyl may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to amine oxides, cocoalkyldimethyl in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, amine oxides, cocoalkyldimethyl is readily biodegradable and does not persist in the environment. In an OECD 301 D test, degradation was 89% after 14 days and 93% after 28 days (OECD, 2006).

[2] OECD, 2006

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, amine oxides, cocoalkyldimethyl is moderately toxic to aquatic organisms. Based on hazard data, freshwater green algae are considered the most sensitive species, for acute and chronic endpoints. Acute toxicity is affected by chain length for fish and invertebrates.

Amine oxides, cocoalkyldimethyl is readily biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for amine oxides, cocoalkyldimethyl are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNEC for water (see **Table 3**). There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method (see **Tables 4 and 5**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site

DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of amine oxides, cocoalkyldimethyl in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, first, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The concentration of amine oxides, cocoalkyldimethyl within the stimulation fluids will decrease in response to biodegradation and photolytic degradation of constituents over time. Chemical-specific biodegradation information presented in the dossier was used for the assessment.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

References

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Attachment 1 Risk Assessment Dossier

AMINE OXIDES, COCOALKYLDIMETHYL

This dossier on amine oxides, cocoalkyldimethyl presents the most critical studies pertinent to the risk assessment of amine oxides, cocoalkyldimethyl in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on amine oxides (OECD, 2006). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Amine oxides, cocoalkyldimethyl was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Amine oxides, cocoalkyldimethyl was assessed as a tier 2 chemical for acute and chronic toxicity of fish and invertebrates, a tier 3 chemical for acute and chronic toxicity of algae. Based on its potential for rapid degradation in the environment, it is not expected to pose a substantial toxic concern to environmental receptors. Therefore, amine oxides, cocoalkyldimethyl are classified overall as **tier 2** chemicals and require a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Amine oxides are surfactants commonly used in consumer products such as shampoos, conditioners, detergents, and hard surface cleaners. Alkyl dimethyl amine oxide (chain lengths C10–C16) is the most commercially used amine oxide. They serve as stabilizers, thickeners, emollients, emulsifiers, and conditioners with active concentrations in the range of 0.1–10 percent (%). The remainder (< 5%) is used in personal care, institutional, commercial products and for unique patented uses.

Amine oxides, cocoalkyldimethyl is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for absorption to soil and sediment.

In general, amine oxides, cocoalkyldimethyl does not exhibit significant acute oral or dermal toxicity. It appears to be a skin and eye irritant but it is not a skin senistiser. It is not a reproductive or developmental toxicant, genotoxic or expected to be a carcinogen. Overall, amine oxides, cocoalkyldimethyl is moderately toxic to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name: Coco alkyldimethylamine oxides

CAS RN: 61788-90-7

Molecular formula: $CH_3.(CH_2)_R.N(CH_3)_2$:O where R is 9-17 (UVCB substance)

Molecular weight: Unspecified (UVCB substance)

Synonyms: Cocamine oxide; coco dimethylamine oxide; coconutdimethylamineoxide; N-(cocoalkyl)-dimethylamine oxide; N,N-dimethylcocamino oxide.

3 PHYSICO-CHEMICAL PROPERTIES

Specific physico-chemical properties on amine oxides, cocoalkyldimethyl are unavailable. Therefore, key physical and chemical properties for the surrogate substance Amines, C10-16-Alkyldimethyl, N-oxides, Average Chain Length 12.6* (CAS No. 70592-80-2), are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Amines, C10-16- Alkyldimethyl, N-oxides, Average Chain Length 12.6* [CAS No. 70592-80-2] (OECD, 2006)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid (commercially available in water at 25-35% activity)	-	OECD, 2006
Melting point	Average: 130.5°C (pressure not provided)	2	OECD, 2006
Boiling point	Decomposes before boiling***	2	OECD, 2006
Vapor pressure	Negligible	2	OECD, 2006
Partition coefficient (log K_{ow})	<2.7	2	OECD, 2006
Water solubility	410 g/L	2	OECD, 2006

*Except melting point.

**Aliphatic amine oxides undergo thermal decomposition between 90° and 200°C. So, melting point is likely to be accompanied with decomposition; all boiling points are predicted to be far above the decomposition temperature.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for amine oxides, cocoalkyldimethyl.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Amine oxides, cocoalkyldimethyl is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for absorption to soil and sediment.

B. Biodegradation

Amine oxides, cocoalkyldimethyl is readily biodegradable. In an OECD 301 D test, degradation was 89% after 14 days and 93% after 28 days (OECD, 2006) [Kl. score = 2].

If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for amine oxides, cocoalkyldimethyl. Based on read-across from amines, C12-14 (even numbered)-alkyldimethyl, N-oxides (CAS No. 308062-28-4), a normalised organic carbon to water partition coefficient (K_{oc}) value of 1,525 L/kg was identified (ECHA). Based on this estimated value, amine oxides, cocoalkyldimethyl is expected to have low mobility in soil. If released to water, based on the K_{oc} value and its water solubility, it is expected to adsorb to suspended solids and sediment.

D. Bioaccumulation

There are no bioaccumulation studies on amine oxides, cocoalkyldimethyl. Amine oxides, cocoalkyldimethyl is not expected to bioaccumulate based on a log n-octanol/water partition coefficient (K_{ow}) of <2.7 (OECD, 2006).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

In general, amine oxides, cocoalkyldimethyl does not exhibit significant acute oral or dermal toxicity. It appears to be a skin and eye irritant but it is not a skin senistiser. It is not a reproductive or developmental toxicant, genotoxic or expected to be a carcinogen.

B. Toxicokinetics/Metabolism

Following an oral dose to male and female rats, approximately 75% of the radioactivity was excreted within 24 hours. Excretion was primarily in the urine (>50%), followed by feces and expired CO_2. The amount of test compound recovered in liver was 1.1 to 1.5%; 1.9 to 4.8% of the dose was retained in the carcass, with the remaining tissues ≤0.1% of the dose. Degradation of the alkyl chain to 4-carbon acid metabolites was more efficient in rabbits (OECD, 2006).

In two human volunteers, the uptake and excretion of 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5) was rapid, with 37 to 50% of the administered radioactivity collected in urine and 18

to 22% in the expired air within two hours after dosing. Humans were more efficient than rats in metabolizing the alkyl chain to 4-carbon acid metabolites (Turan and Gibson, 1981).

C. Acute Toxicity

Oral

The oral LD_{50} in rats of amine oxides, cocoalkyldimethyl was 1,236 mg/kg in males and 846 in females (OECD, 2006) [Kl. score = 2]. In another study, the oral LD_{50} in rats of amine oxides, cocoalkyldimethyl was 3,873 mg/kg (OECD, 2006) [Kl. score = 2].

Inhalation

No inhalation studies available.

Dermal

The dermal LD_{50} values of amines, C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) were >520 mg/kg (OECD, 2006) [Kl. score = 2].

D. Irritation

Application of amine oxides, cocoalkyldimethyl (30% solution) to the skin of rabbits for 4 hours under semi-occlusive conditions was irritating (OECD, 2006 [Kl. score = 1].

Instillation of a 30% solution of 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5) into the eyes of rabbits was slightly irritating (OECD, 2006) [Kl. score = 2].

Instillation of 28% solution of C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) into the eyes of rabbits was moderately to severely irritating (OECD, 2006) [Kl. score = 2]. In another study, Instillation of 27.84% solution of C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) into the eyes of rabbits was moderately irritating (OECD, 2006) [Kl. score = 2].

E. Sensitization

No studies are available on amine oxides, cocoalkyldimethyl.

C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) was not considered to be a skin senistiser in a guinea pig Buehler test (OECD, 2006) [Kl. score = 2].

F. Repeated Dose Toxicity

No studies are available on amine oxides, cocoalkyldimethyl.

Oral

Male and female SD rats were given in their diet 0, 0.1, 0.2, or 0.4% C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) for 13 weeks. The estimated daily intakes were: 0, 63, 112, and 236 mg/kg-day for males; and 0, 80, 150, and 301 mg/kg-day for females. Mean body weights were significantly

lower in the 0.4% males and ≥0.2% females. The opthalmoscopic examination showed lenticular opacities in the posterior cortex of the ≥0.2% males. There were no treatment-related effects in the clinical chemistry and hematology parameters; nor was there any histopathologic changes in the treated animals compared to controls. The NOAEL for this study is 0.1% in the diet, which corresponds to 63 and 80 mg/kg-day for males and females, respectively (OECD, 2006) [Kl. score = 2].

Male and female New Zealand rabbits were given in their diet 0, 0.1, 0.5, or 1.0% C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) for 32 weeks. The estimated daily intakes were: 0, 40, 196, and 390 mg/kg-day for males; and 0, 39, 195, and 380 mg/kg-day for females. There were no opthalmoscopic effects. The 0.5% males had decreased alkaline phosphatase levels and increased relative liver weights. Histopathologic examination showed no treatment-related effects. The NOAEL for this study is 1% in the diet, which corresponds to 40 and 39 mg/kg BW/day for males and females, respectively (OECD, 2006) [Kl. score = 2].

Male and female rats were given in their diet 0, 0.1, 0.1, or 0.2% C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) for 104 weeks. The estimated daily intakes were: 0, 4.24, 42.3, or 87.4 mg/kg-day for males; and 0, 5.23, 52.6, or 107 mg/kg-day for females. Survival, clinical chemistry, opthalmoscopic exams, clinical signs, gross pathology, and histopathology were similar across groups. The 0.2% animals had reduced body weights of >10%. The NOAEL for this study is 0.1% in the diet, which corresponds to 42 and 53 mg/kg-day for males and females, respectively (OECD, 2006) [Kl. score = 2].

Inhalation

No studies are available.

Dermal

Male and female ICR Swiss mice received dermal applications of an aqueous solution of C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) 3 times/week for 104 weeks. The average daily dose was 0, 1.1, 2.8, or 5.6 mg/kg-day. The high-dose mice showed microscopic signs of skin irritation. There were no other treatment-related effects (OECD, 2006) [Kl. score = 2].

G. Genotoxicity

In Vitro Studies

The in vitro genotoxicity studies on amine oxides, cocoalkyldimethyl and similar substances are shown in Table 3.

Table 3 *In vitro* Genotoxicity Studies on Amine Oxides, Cocoalkyldimethyl

Test System	Results**		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	2	ECHA
Mammalian cell gene mutation (Chinese hamster fibroblasts)**	-	-	1	ECHA

*+, positive; -, negative

**Read-across from C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2).

In Vivo Studies

In a dominant lethal test, male mice were given in their drinking water 0, 10, 100, or 1,000 mg/kg 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5). There was no evidence of a mutagenic effect (OECD, 2006) [Kl. score = 2].

H. Carcinogenicity

No carcinogenicity studies are available on amine oxides, cocoalkyldimethyl.

Oral

Male and female rats were given in their diet 0, 0.1, 0.1, or 0.2% C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) for 104 weeks. The estimated daily intakes were: 0, 4.24, 42.3, or 87.4 mg/kg-day for males; and 0, 5.23, 52.6, or 107 mg/kg-day for females. The incidence of tumors was similar between treated and control animals (OECD, 2006) [Kl. score = 1].

Dermal

Male and female ICR Swiss mice received dermal applications of an aqueous solution of C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) 3 times/week for 104 weeks. The average daily dose was 0, 1.1, 2.8, or 5.6 mg/kg-day. The high-dose mice showed microscopic signs of skin irritation. There was no evidence of skin tumors at any dose level (OECD, 2006) [Kl. score = 2].

I. Reproductive Toxicity

A two-generation reproductive toxicity study has been conducted in CD rats on 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5). The dietary levels were 0, 750, 1,500, and 3,000 ppm for 6.5 weeks, and 0, 188, 375, and 750 ppm for the remainder of the study. The dietary levels were reduced because of the reduced body weight gain in the mid- and high-dose groups. There were slight reductions in body weight gain of both the parental animals and offspring, but mating performance and fertility were unaffected by treatment in either generation. Macroscopic and microscopic pathologic examinations showed no differences between treated and control groups. The NOAEL for reproductive and developmental toxicity is 750 ppm, which corresponded to 40 mg/kg-day (OECD, 2006) [Kl. score = 1].

J. Developmental Toxicity

Pregnant female CD rats were dosed by oral gavage with 0, 50, 100, or 200 mg/kg 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5) on GD 7 to 17. One-half of the females/group were sacrificed on GD 20, and the other half were allowed to deliver; the pups were weaned at PND 25 and the F_1 animals were paired at 10 weeks of age. Body weights and water consumption were lower (<10%) in the 200 mg/kg group. Mean fetal weights were lower and associated with slight retardation of fetal ossification in the 200 mg/kg group that were sacrificed in GD 20. However, pup survival and pup growth were unaffected in the offspring of the 200 mg/kg group that were allowed to deliver. The subsequent growth, mating performance, and fertility of the F_1 animals were similar between treated and control groups; F_1 females from the 200 mg/kg F_0 group had slightly elevated fetal and placental weights. There were no macroscopic changes seen in the F_1 animals at terminal necropsy that were considered to be treatment-related. The NOAEL for maternal and developmental toxicity is 100 mg/kg-day (OECD, 2006) [Kl. score = 1] suggesting that observations of developmental toxicity are related to maternal effects.

Pregnant female SD rats were dosed by oral gavage with 0, 25, 100, or 200 mg/kg C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) on GD 6-19. There was one death in the 200 mg/kg group. The $\geq$100 mg/kg groups had reduced body weight gain and relative feed consumption. In the 200 mg/kg group, early resorptions were increased, and liver litter sizes and fetal body weights were decreased. The reduced fetal body weights were associated with fetal variations consisting of delays in skeletal ossifications. The 100 mg/kg group also showed some delays in ossification. There was no indication of fetal malformations at any dose level. The NOAEL for maternal and developmental toxicity is 25 mg/kg-day (OECD, 2006) [Kl. score = 2] suggesting that observations of developmental toxicity are related to maternal effects.

Pregnant female New Zealand rabbits were dosed by oral gavage with 0, 40, 80, or 160 mg/kg 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5) on GD 6-18. Three of the 80 mg/kg and three of the 160 mg/kg dams died or were killed in extremis; these deaths were not considered to be treatment-related. Body weight gain was reduced in all treated groups, although 40 mg/kg dams achieved similar body weights to controls at study termination. Feed consumption was reduced compared to the pre-treatment period during the second half of the treatment period in the 40 and 80 mg/kg animals and for the entire treatment period in the 160 mg/kg animals. Water consumption was also decreased in all treated groups. There was no indication of developmental toxicity. The NOAEL for maternal toxicity was considered to be > 160 mg/kg-day based on decreased body weight. The NOAEL for developmental toxicity is > 160 mg/kg-day, the highest dose tested (OECD, 2006) [Kl. score = 1].

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for amine oxides, cocoalkyldimethyl follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

In a two-year rat dietary study, the lowest NOAEL was 42 mg/kg-day (OECD, 2006). The NOAEL of 42 mg/kg-day will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 42/(10 x 10 x 1 x 1 x 1) = 42/100 = 0.4 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.42 x 70 x 0.1)/2 = 1.5 mg/L

Cancer

There are no carcinogenicity studies on amine oxides, cocoalkyldimethyl. However, C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) was not carcinogenic to rats in a 2-yr dietary study; nor was there any evidence of skin tumors in mice in a 104-week dermal study. Thus, a cancer reference value was not derived.

L. Human Health Hazard Assessment of Physico-Chemical Properties

Amine oxides, cocoalkyldimethyl does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Overall, amine oxides, cocoalkyldimethyl is moderately toxic to aquatic organisms. Based on hazard data, freshwater green algae are considered the most sensitive species, for acute and chronic endpoints. Acute toxicity is affected by chain length for fish and invertebrates.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on amine oxides, cocoalkyldimethyl.

Table 4 Acute Aquatic Toxicity Studies on Amine Oxides, Cocoalkyldimethyl

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Salmo gairdneri	96-hr LC_{50}	13	1	OECD, 2006
Brachydanio rerio	96-hr LC_{50}	1.0	2	OECD, 2006
Leuciscus idus melanotus	96-hr LC_{50}	4.3	2	OECD, 2006
Daphnia magna	48-hr EC_{50}	2.9	1	OECD, 2006
Selenastrum capricornutum	72-hr EC_{50}	0.29	2	OECD, 2006

Chronic Studies

The 302-d NOEC for C10-16 alkyldimethyl, N-oxides (CAS No. 70592-80-2) to *Pimephales promelas* was 0.42 mg/L; this value is 0.31 mg/L when normalized to a $C_{12.9}$ amine oxide (OECD, 2006) [Kl. score = 2].

The 21-day NOEC for 1-dodecanamine, N,N-dimethyl-, N-oxide (CAS No. 1643-20-5) in a *Daphnia* reproduction test is 0.36 mg/L; this value is 0.28 mg/L when normalized to a $C_{12.9}$ amine oxide (OECD, 2006) [Kl. score = 1].

As noted with acute toxicity, green algae are the most sensitive for chronic endpoints, with a 72-hr EC_{20} value of 0.09 mg/L for *Selenastrum capricornutum*. (The geometric mean of 12 studies for the group was 0.11 mg/L) (OECD, 2006) [Kl. score = 2].

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for amine oxides, cocoalkyldimethyl follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C50 values are available for fish (1.0 mg/L), invertebrates (2.9 mg/L), and algae (0.29 mg/L). Results from chronic studies are available for fish (0.31 mg/L), invertebrates (0.28 mg/L), and algae (0.09 mg/L). On the basis that the data consists of short-term and long-term studies for three trophic levels, an assessment factor of 10 has been applied to the lowest reported NOEC value of 0.09 mg/L for algae. The $PNEC_{water}$ is 0.009 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, a $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.21 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 30.08/1280 \times 1000 \times 0.009$
$= 0.2115$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = 0.009 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 61)/1000 \times 2400]$
$= 30.08\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 1525 \times 0.04$
$= 61$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for amine oxides, cocoalkylmethyl is 1525 L/kg based on read-across from C12-14 (even numbered)-alkyldimethyl, N-oxides (CAS No. 308062-28-4) (ECHA).
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.18 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (30.5/1500) \times 1000 \times 0.009$
$= 0.18$ mg/kg dw

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 kg/m^3 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 1525 \times 0.02$
$= 30.5\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for amine oxides, cocoalkylmethyl is 1525 L/kg based on read-across from C12-14 (even numbered)-alkyldimethyl, N-oxides (CAS No. 308062-28-4) (ECHA).
F_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2017).

Amine oxides, cocoalkyldimethyl is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a predicted log K_{ow} of <2.7, amine oxides, cocoalkyldimethyl does not meet the screening criteria for bioaccumulation.

The lowest NOEC from chronic aquatic toxicity studies conducted on amine oxides, cocoalkyldimethyl and similar substances is <0.1 mg/L. Thus, amino oxides, cocoalkyldimethyl meets the screening criteria for toxicity.

The overall conclusion is that amine oxides, cocoalkyldimethyl is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for amine oxide cocoalkyldimethyl.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Amine oxides cocoalkyldimethyl	61788-90-7	Not a PBT	No	No	No	No	No	Yes	2 (fish, inv) 3 (algae)	2 (fish, inv) 3 (algae)	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

CAS No. = chemical abstracts service number

COC = chemical of concern

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
CAS No.	Chemical Abstracts Service Number (also referred to as CAS RN)
COC	chemical of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC_{50}	median effective concentration
ECHA	European Chemicals Agency
EU	European Union
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC_{50}	lethal concentration 50%
LD_{50}	lethal dose 50%
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration

ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Dataset
TG	Test Guideline
USEPA	United States Environmental Protection Agency

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
					0	30	0	30	0	30	
Amine Oxides, cocoalkyldimethyl	61788-90-7	7.90E+00	1.50E+01	1.05E+00	1.05E-01	2.63E-02	1.05E-03	2.63E-04	2.11E-05	5.27E-06	9.00E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Ammonium Hydroxide

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Ammonia (CAS No. 7664-41-7) dissolves readily in water to form the solution described as ammonium hydroxide (CAS No. 1336-21-6). Ammonium Hydroxide is a component in the Water Management Facility (WMF) product used as a disinfectant during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Ammonium hydroxide Water	1336-21-6 7732-18-5	Disinfectant	2 x 1000 L (IBC)

CAS No = Chemical Abstracts Service Number
IBC = intermediate bulk container
L = litre

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Since an Australian Drinking Water Guideline (ADWG) Value is available for ammonia (see **Table 2**), toxicological reference values (TRVs) were not derived for the chemical. A detailed discussion of the drinking water guideline values is presented in the risk assessment dossier provided in **Attachment 2**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Ammonia (7664-41-7)	Ammonia	0.5 mg/L (aesthetics)

CAS No = Chemical Abstracts Service Number mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of TRVs was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observed effect concentration (NOEC) (mg/L), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to **Attachment 2** regarding the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Ammonia (7664-41-7)	-	-	-	0.9[a]

[a] $PNEC_{water}$ for ammonia is the ANZG Water Quality Guideline – Freshwater Trigger Value for total ammonia-N.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

The molecular structure of ammonium hydroxide is presented in **Figure 1** below.

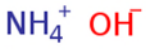

Figure 1 Molecular Structure of Ammonium Hydroxide[2]

Ammonium hydroxide is a solution of ammonia in water. The term 'ammonia' refers to two chemical species of ammonia that are in equilibrium in water: the un-ionised ammonia, NH_3, and the ionised ammonium ion, NH_4^+. The proportion of the two chemical forms in water varies with the physico-chemical properties of the water, particularly pH and temperature. Under environmental conditions (pH 5-8), the predominant form will be the ammonium ion (NH_4^+). As a result, hereafter within this assessment, the term ammonia refers to ammonium hydroxide, ammonia or the ammonia/ammonium ion.

Ammonia is rapidly converted to nitrate by nitrification under aerobic conditions in the aquatic environment. Ammonia is part of the nitrogen cycle. Biodegradation is not applicable to ammonia. Ammonia is easily mineralised to the nitrite ion (NO_2^-) by numerous species of bacteria. Ammonia is not expected to bioaccumulate in the environment because of its dissociation to the ammonium ion and because it is part of the nitrogen cycles in air, soil and water. Ammonia has a low potential to adsorb to soil and sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for ammonia is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the chemical is not a PBT substance.

Human Health Hazards

Ammonia has a moderate acute toxicity by the inhalation route. Depending on the concentration, solutions of ammonia are corrosive, irritating or non-irritating. These solutions cause direct effects to the skin, eyes, respiratory tract and gastrointestinal tract. Vapours from aqueous solutions of ammonia can cause respiratory irritation.

No systemic, reproductive or developmental toxicity was seen in rats at oral doses up to 1,500 milligrams per kilogram-day (mg/kg-day) diammonium phosphate in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Ammonia is not genotoxic.

TRVs were not derived for ammonia. The ADWG value for ammonia is 0.5 milligrams per litre (mg/L) based on aesthetics (see **Table 2**). A detailed discussion f the drinking water guideline values is presented in **Attachment 2**.

Based on the treatment process described in **Attachment 1**, residual ammonia would be present in treated water (permeate) but is not directed to the brine pond. Managed release of treated water to

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/startswith/1336-21-6

the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for human receptors to be exposed to ammonia in Dawson River discharge. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, ammonia is moderately toxic to a variety of aquatic and terrestrial organisms on both an acute and chronic basis. In general, the effect concentration is on the order of a low to mid part per million range. The chronic no observable effect concentrations (NOECs) reported in ANZG (2018) for ammonia for aquatic species are greater than 1 mg/L, except for a mollusc found in New Zealand. It is unknown whether a similar sensitive species is found in Australia.

Ammonia is part of the nitrogen cycle. Biodegradation is not applicable to ammonia or the ammonium ion. Ammonia is also not expected to bioaccumulate in the environment because of its dissociation to the ammonium ion.

The ANZG (2018) for ammonia in freshwaters is: "A freshwater high reliability trigger value of 900 µg/L TOTAL ammonia-N was calculated at pH 8.0 [emphasis added] using the statistical distribution method with 95% protection. This translates to about 900 µg/L un-ionised ammonia-N at 20°C." Considering the land uses adjacent to the Dawson River include light to moderate grazing, and there is some development upstream of the Horseshoe Lakes, adoption of the 95% species protection criteria is considered appropriate (AECOM, 2019).

No experimental toxicity data on sediment or soil organisms are available. Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics, such as ammonia or the ammonium ion. Thus, the equilibrium partitioning method cannot be used to calculate PNECs for soil or sediment. Based on its properties, ammonia and the ammonium ion are not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, estimated permeate concentrations in released treated water (0.0175 mg/L, refer **Attachment 2**) are less than the ANZG freshwater quality guideline value of 0.9 mg/L.

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Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Ammonium Hydroxide 10-35%	Ammonium Hydroxide Water	1336-21-6 7732-18-5	10-35% 65-90%	Ammonia Aqueous Solution	REDOX	Reverse Osmosis Plant	1000L (IBC)	20%	2 x 1000L (IBC)	20%	2 mg/L (AVG)	20%	7300L	used to form monochloramine / disinfectant

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		Brine Concentration	
				(mg/L)	Permeate notes	(mg/L)	Brine Notes
Ammonium Hydroxide 10-35%	Ammonium Hydroxide	1336-21-6	Unreacted / residual ammonia to Desalinated Water Balance Pond	0.0175	Will stay as ammonia or ammonium (NH4+) and approximately 50:50. Therefore, residual ammonia = 2 mg/L * 35%*0.5 = 0.35 mg/L. At a rejection efficiency of 95%, the estimated concentration of ammonia in the permeate is 0.0175 mg/L.	NA	Not directed to brine pond
	Water	7732-18-5		NA		NA	

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

AMMONIA (CAS NO. 7664-41-7)
AMMONIUM HYDROXIDE (CAS NO. 1336-21-6)

This dossier on ammonia and ammonium hydroxide presents the most critical studies pertinent to the risk assessment of ammonia and ammonium hydroxide in their use in water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA) and the OECD-SIDS category for ammonia (OECD, 2007). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ammonia and ammonium hydroxide were not identified in chemical databases used by NICNAS as an indicator that the chemicals are of concern and are not a PBT substance. Ammonia and ammonium hydroxide was assessed as tier 2 chemicals for acute and chronic toxicity. Therefore, ammonia and ammonium hydroxide are classified overall as **tier 2** chemicals and require a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Ammonia (CAS No. 7664-41-7) dissolves readily in water to form the solution described as ammonium hydroxide (CAS No. 1336-21-6). In water, ammonia is in equilibrium with the ammonium ion (NH_4^+), depending on the pH. Under environmental conditions (pH 5-8), the predominant form will be the ammonium ion (NH_4^+).

Ammonia or ammonium ion is rapidly converted to nitrate by nitrification under aerobic conditions in the aquatic environment. Ammonia is part of the nitrogen cycle. Biodegradation is not applicable to ammonia or the ammonium ion. Ammonia (or the ammonium ion) is easily mineralised to the nitrite ion (NO_2^-) by numerous species of bacteria. Ammonia is not expected to bioaccumulate in the environment because of its dissociation to the ammonium ion and because it is part of the nitrogen cycles in air, soil and water. Ammonia and the ammonium ion have a low potential to adsorb to soil and sediment.

The acute toxicity of ammonia is moderate by the inhalation route. Depending on the concentration, solutions of ammonia are corrosive, irritating or non-irritating. These solutions cause direct effects to the skin, eyes, respiratory tract and gastrointestinal tract. Vapours from aqueous solutions of ammonia can cause respiratory irritation. No target organ effects were seen in rats given ammonia by oral gavage or in feed for up to two years. Ammonia is not genotoxic. There were no increases in tumours when rats were fed ammonia in their diet for two years. A reproductive and developmental screening toxicity (OECD 422) study showed no reproductive or developmental effects in rats when given oral gavage doses of an aqueous solution of ammonia.

Ammonia is acutely toxic to aquatic life. The ANZG guidelines for fresh and marine water quality (ANZG, 2018) has a freshwaters trigger value of 900 µg/L TOTAL ammonia-N at pH 8.0.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Ammonia
CAS RN: 7664-41-7
Molecular formula: NH_3
Molecular weight: 17 g/mol

Synonyms: Ammonia, ammonia gas, ammonia anhydrous, liquid ammonia

Chemical Name (IUPAC): Ammonium Hydroxide
CAS RN: 1336-21-6
Molecular formula: H_5NO or NH_4OH
Molecular weight: 35.05 g/mol

Synonyms: Ammonia, aqueous solution; aqua ammonia; ammonia, monohydrate; ammonia liquor; ammonia water

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substances are shown in Tables 1 and 2.

Table 1 Overview of the Physico-chemical Properties of Ammonia

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless gas	2	ECHA
Melting Point	-77.7°C @ 101.3 kPa	2	ECHA
Boiling Point	-33.15°C @ 101.3 kPa	2	ECHA
Vapour Pressure	861,100 Pa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	0.23 @ 20 °C	-	ECHA
Water Solubility	482 g/L @ 25°C	2	ECHA
Dissociation constant (pKa)	9.25@ 25°C	2	ECHA

Table 2 Overview of the Physico-chemical Properties of Ammonium Hydroxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless aqueous solution	-	PubChem
Melting Point	-77°C @ 101.3 kPa	2	OECD, 2007
Boiling Point	-36°C, pressure not specified	4	OECD, 2007
Vapour Pressure	287,800 Pa @ 20°C	2	OECD, 2007
Partition Coefficient (log K_{ow})	Not applicable	-	OECD, 2007
Water Solubility	Miscible	2	OECD, 2007
Dissociation constant (pKa)	10.6-11.6 @ 25°C	2	OECD, 2007

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 3). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No other specific environmental regulatory controls or concerns were identified within Australia and internationally for ammonia.

NICNAS has assessed ammonium hydroxide in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment. It is a reactive substance which rapidly converts into species of low ecotoxicological concern. This chemical, and its degradant species, are not expected to pose an unreasonable risk to the environment provided that ANZECC water quality guidelines for physical and chemical stressors are not exceeded[1].

Table 3 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Ammonium hydroxide is a solution of ammonia in water. The term 'ammonia' refers to two chemical species of ammonia that are in equilibrium in water: the un-ionised ammonia, NH_3, and the ionised ammonium ion, NH_4^+. The proportion of the two chemical forms in water varies with the physico-chemical properties of the water, particularly pH and temperature.

The following equilibria occurs at ambient environmental conditions:

$NH^+ + H_2O \leftrightarrow NH_3 + H^+$
$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$

Under environmental conditions (pH 5-8), the predominant form will be the ammonium ion (NH_4^+). As pH decreases, the concentration of the ammonium ion will increase, while the un-ionised ammonia concentration will decrease.

Ammonia is volatile and once exposed to open air, liquid ammonia quickly turns into a gas and forms ammonia gas. Ammonia is a colourless gas at room temperature and pressure. Gas-phase ammonia

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=1336-21-6

will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and nitrate radicals (PubChem).

Ammonia is very soluble in water, the solubility being around 482 g/L at 25°C. Ammonia or ammonium ion is rapidly converted to nitrate by nitrification under aerobic conditions in the aquatic environment (OECD, 2007). Ammonia is part of the nitrogen cycle. Biodegradation is not applicable to ammonia or the ammonium ion. Ammonia (or the ammonium ion) is easily mineralised to the nitrite ion (NO_2^-) by numerous species of bacteria (OECD, 2007).

Ammonia is not expected to bioaccumulate in the environment because of its dissociation to the ammonium ion and because it is part of the nitrogen cycles in air, soil and water. Ammonia and the ammonium ion have a low potential to adsorb to soil and sediment.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of ammonia is moderate by the inhalation route. Depending on the concentration, solutions of ammonia are corrosive, irritating or non-irritating. These solutions cause direct effects to the skin, eyes, respiratory tract and gastrointestinal tract. Vapours from aqueous solutions of ammonia can cause respiratory irritation. No target organ effects were seen in rats given ammonia by oral gavage or in feed for up to two years. Ammonia is not genotoxic. There were no increases in tumours when rats were fed ammonia in their diet for two years. A reproductive and developmental screening toxicity (OECD 422) study showed no reproductive or developmental effects in rats when given oral gavage doses of an aqueous solution of ammonia.

B. Acute Toxicity

The oral LD_{50} of aqueous ammonia (as ammonium hydroxide) in rats is 350 mg/kg (Smyth et al., 1941). [Kl. score = 2]

The 1-hour LC_{50} values of ammonia in rats are 9,850 mg/m^3 for males and 13,770 mg/m^3 for females (Appelman et al., 1982). [Kl. score = 2]

C. Irritation

Application of a 12% aqueous solution of ammonia (as ammonium hydroxide) to the skin of rabbits for four hours under occlusive conditions was corrosive. A 10% aqueous solution was not corrosive under similar conditions (ECHA). [Kl. score = 2]

No eye irritation studies are available.

D. Sensitisation

No studies are available.

E. Repeated Dose Toxicity

Oral

In a combined repeated dose toxicity study with the reproduction/developmental toxicity screening test (OECD 422), male and female Crj: CD(SD) male and female rats were dosed by oral gavage with 0, 250, 750 or 1,500 mg/kg diammonium phosphate. The exposure period for the toxicity subgroup was 35 days. There was no treatment-related deaths and no clinical signs of toxicity. The 1,500 mg/kg males had reduced (22% of controls) body weight gain and feed consumption. Activated partial thromboplastin time was reduced in the 750 and 1,500 mg/kg males. In males: elevated alkaline phosphatase (750 and 1,500 mg/kg; 132% and 131% of controls); reduced glucose and phosphorus levels (1,500 mg/kg; 79% and 82% of controls); reduced total protein (750 and 1,500 mg/kg; 93% and 91% of controls); slightly elevated albumin/globulin ratio (1,500 mg/kg; 117% of controls). In females: decreased phosphorus levels (1,500 mg/kg; 81% of controls). No details were given as to whether these values were within normal range. The functional observation battery (FOB) and motor activity results showed no treatment-related effects. Relative kidney and liver weights were increased in the 1,500 mg/kg females compared to controls. Reddening of the extremities were seen in all dose groups during the first week of the study but were reduced as the study progressed. Histopathologic examination showed submucosal inflammation of the stomach at all dose levels, which was not statistically significant at 250 mg/kg-day. Given the lack of histopathological findings (excluding the irritation effect seen in stomach), the serum chemistry changes do not seem indicative of an adverse effect. The NOAEL for this study is 750 mg/kg-day (ECHA). [Kl. score = 1]

Male and female F344 rats were fed in their diet 0, 0.1, 0.6 or 3% ammonium sulfate for 52 weeks. The estimated daily intakes were: 0, 42, 256 and 1,527 mg/kg-day for the males; and 0, 48, 284 and 1,490 mg/kg-day for the females. There was a significant increase in kidney and/or liver weights in the 3% dietary group. No effects were noted for survival, body weights, hematology, serum chemistry, or histopathology. The kidney and liver weight changes do not appear to be an adverse effect because of no corresponding serum chemistry and/or histopathological changes in these organs. The NOAEL for this study is 3% in the diet, corresponding to 1,527 and 1,490 mg/kg-day for males and females, respectively (Ota et al., 2006). [Kl. score = 2]

Male and female F344 rats were fed in their diet 0, 1.5 or 3% ammonium sulfate for 104 weeks. The estimated daily intakes were: 0, 564 and 1,288 mg/kg-day for the males; and 0, 650 and 1,371 mg/kg-day for the females. Body weights and feed consumptions were similar across all groups. There was an increased incidence of chronic nephropathy in the male rats, which was statistically significant only in the 1.5% dietary group (Ota et al., 2006). [Kl. score = 2]

Inhalation

The study of ammonia exposure in workers in a soda ash plant with support from three studies in urea fertilizer plants was identified as the principal study for the derivation of an inhalation reference concentration (RfC). Respiratory effects, characterized as increased respiratory symptoms based on self-report (including cough, wheezing, and other asthma-related symptoms) and decreased lung function in workers exposed to ammonia, were selected as the critical effect. An RfC of 0.5 mg/m^3 was calculated (USEPA, 2016).

Additional information can be found in USEPA's Integrated Risk Information System (IRIS) assessment for ammonia available on-line at:
https://cfpub.epa.gov/ncea/iris2/chemicalLanding.cfm?substance_nmbr=422

Dermal

No studies are available.

F. Genotoxicity

Table 4 lists the *in vitro* genotoxicity studies on ammonia and ammonium sulfate.

In Vitro Studies

Table 4 *In Vitro* Genotoxicity Studies on Ammonia and Ammonium Sulfate

Test System	Test Substance	Results*		Klimisch Score	Reference
		-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* and *E. coli* strains)	Anhydrous ammonia	-	-	2	ECHA
Bacterial reverse mutation (*S. typhimurium* strains)	Ammonium sulfate	-	-	1	ECHA

*+, positive

In Vivo Studies

Male ddY mice were given a single intraperitoneal injection of 0, 62.5, 125, 250 or 500 mg/kg ammonium chloride. There were no increases in the frequency of micronucleated erythrocytes at any dose level (Hayashi et al., 1988).

Male ddY mice were given intraperitoneal injections of 0, 31.3, 62.6, 125 or 250 mg/kg ammonium chloride on four consecutive days. There were no treatment-related increases in the frequency of micronucleated erythrocytes at any dose level (Hayashi et al., 1988).

G. Carcinogenicity

Male and female F344 rats were fed in their diet 0, 1.5 or 3% ammonium sulfate for 104 weeks. The estimated daily intakes were 0, 564 and 1,288 mg/kg-day for the males; and 0, 650 and 1,371 mg/kg-day for the females. Body weights and feed consumptions were similar across all groups. The tumour incidences were similar between the treated and control groups (Ota et al., 2006). [Kl. score = 2]

H. Reproductive/Developmental Toxicity

In a combined repeated dose toxicity study with the reproduction/developmental toxicity screening test (OECD 422), male and female Crj: CD(SD) male and female rats were dosed by oral gavage with 0, 250, 750 or 1,500 mg/kg diammonium phosphate. The males and females were treated for 28 and 53 days, respectively. There were no reproductive or developmental toxicity at any dose level. The NOAEL for reproductive and developmental toxicity is 1,500 mg/kg-day (ECHA). [Kl. score = 1]

I. Derivation of Toxicological Reference and Drinking Water Guidance Values

Non-Cancer

An oral reference dose was not derived for ammonia.

The Australian drinking water guideline value for ammonia (0.5 mg/L, aesthetics) may be applicable (ADWG, 2021).

Cancer

A two-year rat dietary study on ammonium sulfate showed no carcinogenic effects. Thus, a cancer reference value was not derived.

J. Human Health Hazard Assessment of Physico-Chemical Properties

Ammonia is a flammable gas.

It does not exhibit the following physico-chemical properties:

- Explosivity
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Ammonia is moderately toxic to a variety of aquatic and terrestrial organisms. In general the effect concentration is on the order of a low to mid part per million range. Specific data are discussed below.

B. Aquatic Toxicity

ANZG developed a water quality guideline for ammonia (ANZG, 2018). The term 'ammonia' refers to both the un-ionised ammonia (NH_3) and the ionised ammonium ion (NH_4^+). The proportion of the chemical forms in water varies with the physico-chemical properties of the water, particularly pH and temperature. The concentrations of ammonia are usually expressed as either total ammonia (the sum of NH_3 and NH_4^+) which takes into account the total amount as NH_3 or N, or as concentration of the un-ionised NH_3. The concentrations can be given as component of N (e.g., NH_3-N) or total ammonia-N.

The values given below from ANZG (2018) are geometric means of species data taken from all screened data that concurrently measured pH and temperature. Figures were adjusted to a standard pH of 8.0 and calculated in terms of <u>total ammonia-N</u>.

Freshwater fish

The 24 – 96 hour LC_{50} values for 15 species were 3,944 to 169,873 μg/L (an anomalous figure of 72 μg/L was extracted from AQUIRE database [1994]). The 6- to 28-d chronic NOEC and EC_{20} (growth and survival) for 9 species were 1,350 to 19,720 μg/L.

Freshwater crustacean

The 24 – 96 hour LC_{50} values for 10 species are 7,754 to 108,500 μg/L. The cladoceran *Simocephalus vetulus* was the most sensitive (24-hour EC and LC_{50} values were approximately 1,580 μg/L), and the amphipod *Crangonyx pseudogracilis* was the least sensitive. The 7-day to 10-week chronic NOEC and EC_{20} values (reproduction) for 4 species are 1,450 to 19,770 μg/L.

Freshwater insects

The 24 – 96 hour LC_{50} values for eight species are 15,091 to 282,400 μg/L. The 29-day chronic NOEC (reproduction) for two species are 1,790 to 4,400 μg/L.

Freshwater molluscs

The acute toxicity for seven species were 12,588 to 74,623 μg/L. The chronic 42- to 60-day NOEC and EC_{20} (reproduction and survival) for two species are 540 to 2,620 μg/L. The most sensitive species under chronic exposure was the New Zealand species *Sphaerium novaezelandiae* with NOEC (60-day mortality and reproduction) of 540 μg/L total ammonia-N.

Freshwater annelid

The 24 – 96 hour LC_{50} values for two species are 20,071 to 79,788 μg/L.

Freshwater rotifer

The 24-hour LC_{50} for *Brachionus rubens* is 1,300 μg/L.

Freshwater Platyhelminthes

The 24 – 96 LC_{50} value for *Polycelus tenuis* is 37,634 μg/L.

C. Terrestrial Toxicity

At 2.1 to 28 mg/m^3, ammonia gas may damage foliage of plants within four hours; damage may occur within 4 to 8 minutes at air concentrations of 175 to 700 mg/m^3 (WHO, 1986; OECD, 2007). Application of ammonium sulfate to soil inhibited onion growth at 399 mg N/kg soil (OECD, 2007).

Frog species *Pseudacris regilla* and *Rana aurora* exposed to ammonium sulfate in the water for 10 days showed no adverse effects at 17.4 to 82.7 mg NH_3-N/L (OECD, 2007). Larvae of the salamander *Ambystoma gracile* showed no effects after 10 days of exposure to 81.5 mg NH_3-N/L (OECD, 2007).

D. Calculation of PNEC

PNEC water

The ANZG water quality guideline (2018) for ammonia in freshwaters is: "A freshwater high reliability trigger value of 900 μg/L TOTAL ammonia-N was calculated at pH 8.0 [emphasis added] using the statistical distribution method with 95% protection. This translates to about 900 μg/L un-ionised ammonia-N at 20°C." See Appendix for information regarding how the guideline figure changes at different pH values.

PNEC sediment

No experimental toxicity data on sediment organisms are available. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as ammonia and the ammonium ion. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. Based on its properties, no adsorption of ammonia or the ammonium ion to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No experimental toxicity data on soil organisms are available. The environmental distribution of ammonia is dominated by its water solubility. Sorption of ammonia and the ammonium ion should probably be regarded as a reversible situation, *i.e.*, the substance is not tightly nor permanently bound. K_{oc} and K_{ow} parameters do not readily apply to inorganics, such as ammonia or the ammonium ion. Thus, the equilibrium partitioning methods cannot be used to calculate the $PNEC_{soil}$. Based on its properties, ammonia and the ammonium ion are not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Ammonium hydroxide is a solution of ammonia in water. In water, ammonia is in equilibrium with the ammonium ion (NH_4^+), depending on the pH. Under environmental conditions (pH 5-8), the predominant form will be the ammonium ion (NH_4^+). Ammonia or ammonium ion is rapidly converted to nitrate by nitrification under aerobic conditions in the aquatic environment. Ammonia is part of the nitrogen cycle. Biodegradation is not applicable to ammonia or the ammonium ion. Ammonia (or the ammonium ion) is easily mineralised to the nitrite ion (NO_2^-) by numerous species of bacteria. Therefore, ammonia does not meet the criteria for persistence.

Ammonia is not expected to bioaccumulate in the environment because of its dissociation to the ammonium ion and because it is part of the nitrogen cycles in air, soil and water. Thus, ammonia does not meet the criteria for bioaccumulation.

The chronic NOECs reported in ANZG (2018) for ammonia for aquatic species are greater than 0.1 mg/L, except for a mollusc found in New Zealand. It is unknown whether a similar sensitive species is

found in Australia. For the purposes of this risk assessment, the chronic NOECs for ammonia will be considered to be greater than 0.1 mg/L. Acute aquatic toxicity values were greater than 1 mg/L. Thus, ammonia does not meet the screening criteria for toxicity.

The overall conclusion is that ammonia and ammonium hydroxide are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ammonia or ammonium hydroxide.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Ammonia	7664-41-7	Not a PBT	No	No	NA	No	No	No	2	2	2
Ammonium Hydroxide	1336-21-6	Not a PBT	No	No	NA	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

^{o}C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
AQUIRE	Aquatic Toxicity Information Retrieval
atm-m^3mol	atmosphere meter cubed mole
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
FOB	functional observation battery
g/L	grams per litre
hPa	hectopascal
IRIS	Integrated Risk Information System
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
LC	lethal concentration
mg/kg	milligrams per kilogram
mg/m^3	milligrams per cubic metre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration

OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	screening information data set
USEPA	United States Environmental Protection Agency
WHO	World Health Organization
µg/L	micrograms per litre

Appendix

Freshwater trigger values as total ammonia-N in μg/L at different pH (temperature is not taken into consideration). Taken from Table 8.3.7 (ANZG, 2018).

pH	Freshwater Trigger value (mg/L as total ammonia-N)	pH	Freshwater Trigger value (mg/L as total ammonia-N)
6.0	2570	7.6	1470
6.1	2555	7.7	1320
6.2	2540	7.8	1180
6.3	2520	7.9	1030
6.4	2490	8.0	900
6.5	2460	8.1	780
6.6	2430	8.2	660
6.7	2380	8.2	560
6.8	2330	8.4	480
6.9	2260	8.4	400
7.0	2180	8.6	340
7.1	2090	8.7	290
7.2	1990	8.8	240
7.3	1880	8.9	210
7.4	1750	9.0	180
7.5	1610	-	-

Qualitative Tier 2 Assessment

Benzaldehyde

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. . The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Benzaldehyde is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Benzaldehyde	100-52-7	Corrosion Inhibitor	0.00036%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There was no sufficient evidence of carcinogenicity in rat and mouse chronic studies conducted on benzaldehyde. Thus, a cancer reference value was not derived. As a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Benzaldehyde (CAS No. 100-52-7)	Developmental Study	No effects on foetal development	175	1000	0.175	0.61

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Benzaldehyde (CAS No. 100-52-7)	*Pimephales promelas*	0.12	50	0.002

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Benzaldehyde (CAS No. 100-52-7)	[a]	-	-	0.0016

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Benzaldehyde (CAS No. 100-52-7)	[a]	-	-	0.0003

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Benzaldehyde is an aromatic aldehyde bearing a single formyl group with an almond odour. The molecular structure for benzaldehyde is presented in **Figure 1**.

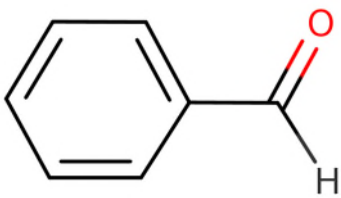

Figure 1 Molecular Structure of Benzaldehyde[2]

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/100-52-7

Benzaldehyde is readily biodegradable. It is not expected to bioaccumulate and has a low potential to adsorb to soil or sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for benzaldehyde is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

Benzaldehyde is hazardous and considered harmful if swallowed, with low acute dermal toxicity and moderate acute inhalation toxicity. It is not irritating to the skin but may be an eye and respiratory irritant. It is not a skin sensitiser. Based on the data available, the chemical is not considered to cause serious damage to health from repeated oral exposure or through inhalation. No data are available to evaluate exposure vie the dermal pathway. The substance is not genotoxic when tested in both in vitro and in vivo assays. There is no indication that this substance will cause malformations or have an adverse effect on reproduction and development.

The half-life of benzaldehyde in the body is short, and that the principal pathway of metabolism of benzaldehyde includes oxidation to yield benzoic acid. Benzoic acid is subsequently conjugated with glycine and excreted as hippuric acid. Sodium benzoate is the sodium salt of benzoic acid, and is also completely metabolized to benzoic acid prior to excretion via the hippuric acid pathway.

In a sub-acute developmental toxicity study conducted in rats and mice using sodium benzoate, dose levels applied showed no evidence of maternal toxicity. No effects on foetal development were reported. A no observed adverse effect level (NOAEL) of 175 mg/kg bw/day was established. This NOAEL was used for determining the oral RfD and the drinking water guideline value (0.61 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Benzaldehyde may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to benzaldehyde in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, benzaldehyde is readily biodegradable and volatilization half-lives for a model river and model lake are 1.5 and 14 days, respectively (PubChem).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km

downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, benzaldehyde has moderate toxicity to aquatic organisms.

Benzaldehyde is readily biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for benzaldehyde are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNECs for water (see **Table 3**). There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method (see **Tables 4 and 5**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at

the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of benzaldehyde in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, first, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The concentration of benzaldehyde within the stimulation fluids will decrease in response to biodegradation and photolytic degradation of constituents over time. Chemical-specific biodegradation information presented in the dossier was used for the assessment.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

BENZALDEHYDE

This dossier on benzaldehyde presents the most critical studies pertinent to the risk assessment of benzaldehyde in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997; Kl).

Screening Assessment Conclusion – Benzaldehyde was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Benzaldehyde was assessed as a tier 2 chemical for acute and chronic toxicity. Therefore, this substance is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Benzaldehyde is an aromatic aldehyde bearing a single formyl group with an almond odour. Benzaldehyde can be derived from natural sources and is widely used by the chemical industry in the preparation of various aniline dyes, perfumes, flavorings, and pharmaceuticals (Pubchem).

Benzaldehyde is readily biodegradable. It is not expected to bioaccumulate. It has a low potential to adsorb to soil or sediment.

Benzaldehyde is hazardous and considered harmful if swallowed, with low acute dermal toxicity and moderate acute inhalation toxicity. It is not irritating to the skin but may be an eye and respiratory irritant. It is not a skin sensitiser. Based on the data available, the chemical is not considered to cause serious damage to health from repeated oral exposure or through inhalation. No data are available to evaluate exposure vie the dermal pathway. The substance is not genotoxic when tested in both *in vitro* and *in vivo* assays. There is no indication that this substance will cause malformations or have an adverse effect on reproduction and development. It has a moderate toxicity to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Benzaldehyde

CAS RN: 100-52-7

Molecular formula: C_7H_6O

Molecular weight: 106.12 g/mol

Synonyms: Artificial Almond Oil;Benzaldehyde FFC; Benzenecarbonal; Benzenecarboxaldehyde;Benzoic aldehyde; Phenylmethanal; Almond artificial essential oil; Phenylmethanal benzenecarboxaldehyde; NCI-C56133; Oil of Bitter Almond;Artificial essential oil of almond; Benzene carbaldehyde;NA 1989; Artificial essential oil of almond; Artificial bitter almond oil; Benzene methylal; Benzoyl hydride; Ethereal oil of bitter almonds; Benzyaldehyde

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Benzaldehyde

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid, becoming yellowish on keeping; almond odor	2	ECHA
Melting point	-26°C @ 101.3 kPa	2	ECHA
Boiling point	179°C @ 101.3 kPa	2	ECHA
Density	1.042 @ 25°C (dimensionless)	2	ECHA
Vapor pressure	169 Pa @ 25°C	2	ECHA
Partition coefficient (log K_{ow})	1.4 @ 25°C	1	ECHA
Water solubility	6.95 g/L @ 25°C	2	ECHA
Dissociation constant (pKa)	14.9 @ 20°C	2	ECHA
Viscosity	1.321 mPa s @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for benzaldehyde.

NICNAS has assessed benzaldehyde in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=100-52-7%2C+

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Benzaldehyde is readily biodegradable. It is not expected to bioaccumulate. It has a low potential to adsorb to soil or sediment.

B. Partitioning

Benzaldehyde is highly soluble in water. Volatilisation from water surfaces or moist soil surfaces is expected to be an important fate process based upon this compound's estimated Henry's Law constant (2.85 Pa m^3/mol). It is also expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

C. Biodegradation

Benzaldehyde is readily biodegradable. In an activate sludge test, degradation was approximately 100% after 19 days as measured by DOC removal (ECHA) [Kl. score = 2].

In a BOD test, degradation was >60% after 28 days as measured by O_2 consumption (ECHA) [Kl. score = 2]. In a CO_2 evolution test, degradation was about 60% in 7 days and 100% in 28 days (ECHA) [Kl. score = 2].

If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for benzaldehyde. Using KOCWIN in EPISUITE™ (EPA, 2019), the estimated K_{oc} value from log K_{ow} is 32.69 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 11.09 L/kg. If released to soil, based on these K_{oc} values, the substance is expected to have very high mobility. If released to water, based on the K_{oc} values and its water solubility, benzaldehyde is not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on benzaldehyde. Benzaldehyde is not expected to bioaccumulate based on a log K_{ow} of 1.4 (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

The following sections detail the available and relevant literature on the toxicity of benzaldehyde. The information described below was obtained from NICNAS IMAP if available and the ECHA database.

A. Summary

Benzaldehyde is hazardous and considered harmful if swallowed, with low acute dermal toxicity and moderate acute inhalation toxicity. It is not irritating to the skin but may be an eye and respiratory

irritant. It is not a skin sensitiser. Based on the data available, the chemical is not considered to cause serious damage to health from repeated oral exposure or through inhalation. No data are available to evaluate exposure vie the dermal pathway. The substance is not genotoxic when tested in both *in vitro* and *in vivo* assays. There is no indication that this substance will cause malformations or have an adverse effect on reproduction and development.

B. Toxicokinetics

The studies of the pharmacokinetics (i.e. absorption, distribution, metabolism and excretion) of benzaldehyde are limited. However, available data provide useful supportive evidence to indicate that the half-life of benzaldehyde in the body is short, and that the principal pathway of metabolism of benzaldehyde includes oxidation to yield benzoic acid. Benzoic acid is subsequently conjugated with glycine and excreted as hippuric acid. In parallel, benzaldehyde is reduced, to a minor extent, to benzyl alcohol, which as the sulfate conjugate may react with glutathione to form benzylmercaturic acid (ECHA) [Kl. Score = 2].

C. Acute Toxicity

Oral

The oral LD50 of the test substance in rats is between 300 and 2000 mg/kg bw/day. In the key OECD 401 Guideline Study (Acute Oral Toxicity) an acute LD50 value for rats appeared to be approximately 1430 mg/kg bw (ECHA) [Kl. Score = 2].

In a supportive study, a LD50 value of 1300 mg/kg bw in rats and 1000 mg/kg bw for guinea pigs was derived. In another limitedly reported supporting study a LD50 value of 800 -1600 mg/kg bw was reported for both rats and mice. In an acute oral toxicity study in rats with the test substance, an oral LD50 of > 2170 mg/kg(> 2000 mg/kg) was reported (ECHA) [Kl. Score = 4].

The chemical is classified as hazardous with the risk phrase 'Harmful if swallowed' (Xn; R22) in HSIS (Safe Work Australia). In humans, a lethal oral dose of 600–900 mg/kg bw was calculated for the chemical in the absence of prompt treatment (NICNAS, 2016).

Dermal

Although limited information is available, the chemical is likely to have low acute dermal toxicity in animal tests following dermal exposure. In the key study, four rabbits were dermally exposed (semi-occlusive) for 24 hours to the test substance (2000 mg/kg). No mortality was observed. The LD50 was considered to be > 2,000 mg/kg bw (ECHA) [Kl. Score = 2]. In an acute dermal toxicity study in rabbits with limited available data, an LD50 of >1250 mg/kg bw was reported (ECHA) [Kl. Score = 4].

Inhalation

Although limited data are available, the available information indicates that the chemical has moderate acute toxicity in animal tests. Based on an acute inhalation toxicity study in rats with the test substance, the inhalation LC50 is 1000 -5000 mg/m^3 (ECHA) [Kl. Score =1].

Based on two studies on sensory irritation (Babiuk 1984, Steinhagen 1983) it cannot be excluded that the test substance induces sensory irritation in rodents. The data are however not sufficient to set an effect level in humans (ECHA) [Kl. Score = 4].

An increased incidence of respiratory symptoms was noted among workers exposed to vapour of the chemical at atmospheric concentrations of >5 mg/m^3 (NICNAS, 2016).

D. Irritation

Although limited data are available, the available information indicates that the chemical is not likely to be a skin irritant but has been reported to be an eye irritant in animal and human studies and a respiratory irritant in humans.

Skin

The shaved skin of guinea pigs was exposed to undiluted benzaldehyde with a gauze pad for 24 hours. The concentration test substance ranged from 5-20 mL/kg. The test substance was moderately irritating to the guinea-pig skin in this test (ECHA) [Kl. Score = 4].

A read-across study was conducted using benzoic acid in New Zealand White Rabbits. The test substance caused very slight erythema in two animals at 60 minutes after removel of the dressings. The erythema had resolved by day 2. Twenty-four hours after test substance removal, one animal showed very slight oedema, which resolved within 24 hours. No signs of systemic intoxication were observed in any of the rabbits. The test substance was considered as minimally irritating to the skin (ECHA) [Kl. Score = 2].

Eyes

In an OECD 405 Guideline Study (Acute Eye Irritation/Corrosion), New Zealand White Rabbits were dosed with 100 microliter of benzaldehyde in the eye and observed for 7 days. The test substance was slightly irritating to the rabbit eye in this test. Immediate irritation effects were noted at one hour and within 24 hours, the anterior portion of the cornea was damaged. The cornea was cleared within 48 hours and only erythema of the conjunctiva and nictitating membrane was noted at this stage. Although the rabbit died on the sixth day, the death was not related to the application of the chemical (ECHA) [Kl. Score = 2].

In an inhalation toxicity study, human volunteers were exposed to 4.5 ppm (19.5 mg/m^3) of the chemical for one minute. Irritation of the eyes and upper respiratory tract were observed. In an occupational study, workers exposed to the chemical vapour at atmospheric concentrations of >5 mg/m^3 reported symptoms of slight eye irritation and considerable skin irritation (NICNAS, 2016).

E. Sensitisation

Overall it is concluded that the test substance is not a skin sensitiser (ECHA).

The test substance was determined not to be a contact sensitiser using the Magnusson-Kligmann method [Kl. Score = 2] and the open epicutaneous test [Kl. Score =4]. However, it was reported positive for allergenicity in guinea pigs in the Draize test, the maximisation test and a test with Freund's complete adjuvant (ECHA) [Kl. Score = 4].

Supportive evidence from Opdyke (1976) showed no evidence of sensitisation in a maximisation test with 25 human volunteers. In this test a concentration of 4% in petrolatum was used. Furthermore, in a human patch test using 5% the test substance in vaseline, positive reactions were noted in 10 of 100 patients. Positive reactions occurred in patients with sensitivity to benzoic acid or vanillin.

Although the chemical has produced skin sensitisation reactions in some tests, based on the weight of evidence, the chemical is not likely to be a skin sensitiser. It is also noted that the chemical is rapidly metabolised to benzoic acid in the skin. Clinical reports of allergy to the chemical are rare and benzoic acid has also been reported not to produce sensitisation in clinical trials in humans (NICNAS, 2016).

F. Repeated Dose Toxicity

Oral

In a sub-chronic oral toxicity study, male and female Fischer 344 rats and B6C3F1 mice were treated daily with the test substance by gavage for 90 days in several doses. Groups of 10 male and 10 female F344 rats were given gavage doses of benzaldehyde of 50, 100, 200, 400 and 800 mg/kg body weight (dissolved in corn oil). Groups of 10 male and 10 female B6C3F1 mice were given benzaldehyde doses of 75, 150, 300, 600 or 1200 mg/kg body weight per day. Both groups were doesd 5 days/week for a period of 13 weeks (90 days).

The symptoms of intoxication observed in the rats of the 800 mg/kg group were increased activity, trembling or periodic inactivity. 6 males and 3 females of this group and 1 female animal of the 400 mg/kg group and the control group died in the second half of the experiment. In the male animals of the 800 mg/kg group, body weight gains and the absolute and relative weights (relative to the brain weight) of the thymus and testes were reduced. The female animals of this group were found to have slightly increased liver, kidney, thymus and heart weights. In most of the animals of the 800 mg/kg group and 2 males of the 400 mg/kg group, slight hyperplasia and hyperkeratosis of the forestomach epithelium, accompanied by increased mitotic activity in the basement membrane, were detected. This study yielded a NOEL for rats of 400 mg/kg body weight per day as the damage to the forestomach is likely due to the application methodology.

No clinical symptoms of intoxication were observed in mice. All male animals and one female from the 1200 mg/kg group died during the first 4 weeks of the experiment. The body weight gains were reduced in the female animals after doses of 1200 mg/kg and in the male animals after doses as low as 600 mg/kg. At the end of the experiment the body weights of the male animals of the 600 mg/kg group were reduced by 9 % relative to those of the controls. The organ weights did not differ from the control values. In the gross pathological and microscopic examinations, weak to moderate degeneration of the renal tubules was detected in all male animals of the 1200 mg/kg group and one male of the 600 mg/kg group. This study therefore yielded a NOEL for male mice of 300 mg/kg body weight per day and for female mice of 600 mg/kg body weight per day (Kluwe et al. 1983, NTP 1990 cited in ECHA) [Kl. Score = 2].

Inhalation

In a short-term inhalation study, groups of 14 Sprague-Dawley rats per sex and group were exposed in whole animal exposure chambers on 14 consecutive days, for 6 hours a day, to benzaldehyde vapour in concentrations of 0, 500, 750 and 1000 mL/m^3 (about 2200, 3300 and 4400 mg/m^3).

During the experiment 11 animals from the 1000 mL/m^3 group died (10 females, 1 male) and 3 female animals from the 750 mL/m^3 group. In all animals exposed to benzaldehyde, tremor, piloerection, diuresis, decreased respiration rates, hypothermia, reduced motor activity and concentration-dependent symptoms of eye and nose irritation occurred in the first week of the experiment. Because effects occurred even at the lowest benzaldehyde concentration of 500 mL/m^3 (2200 mg/m^3), this study did not yield a NOEL (ECHA) [Kl. Score = 2].

In albino rats exposed over a period of 4 months for 5 hours a day to benzaldehyde concentrations of 26 mg/m^3 (about 6.0 mL/m^3) under dynamic conditions, 3 months after the beginning of the experiment changes were detected in haematological parameters (hypoglobulinaemia, erythrocytosis, leukocytosis, initial lymphocytosis followed by lymphopenia) and delays in body weight gain. At the end of the experiment all the parameters were within the normal range (ECHA) [Kl. Score = 4].

Exposure to benzaldehyde concentrations of 6 mg/m^3 (about 1.4 mL/m^3) under otherwise identical conditions was tolerated by albino rats without symptoms (no further details) (Peresedov 1974 cite in ECHA) [Kl. Score = 4].

G. Genotoxicity

Overall, the data indicate that the chemical has no mutagenic or genotoxic potential. Although there is no mutagenic activity in bacterial systems, the chemical does have weak clastogenic effects in some mammalian cell assays.

The genotoxicity of benzaldehyde has been investigated in many in vitro test systems (ECHA). In Salmonella typhimurium, in mutagenicity studies with the strains TA98, TA100, TA102, TA104, TA1535, TA1537 and TA2637, and in a DNA repair test with and without metabolic activation, no genotoxic activity could be detected. In a mutagenicity test with Escherichia coli WP2 uvrA and the mutagen 4-nitroquinoline-1-oxide, benzaldehyde from concentrations of 2120 µg/p1ate was found to have an antimutagenic effect (Watanabe et al. 1988). In Bacillus subtilis, DNA-damaging effects were observed at high concentrations only after metabolic activation. An increase in the incidence of mutants in the mouse lymphoma test occurred only in the high, cytotoxic concentration range and the finding is therefore questionable. Evidence of a weak clastogenic potential in the chromosomal aberration test and in the sister chromatid exchange test was also found only with high concentrations. Therefore, there is merely evidence of weak genotoxic activity of benzaldehyde.

In an *in* vivo test, a sex-linked recessive lethal test with *Drosophila melanogaster*, benzaldehyde administered in a concentration of 1500 ppm with the diet and injection of 2500 ppm was inactive (NTP 1990, Woodruff et al. 1985 cited in ECHA) [Kl. Score = 2].

H. Carcinogenicity

Mammalian data are unclear on the carcinogenicity of benzaldehyde, showing some evidence of carcinogenicity in mice but none in rats. The chemical is also considered not to have mutagenic or genotoxic potential (see Genotoxicity).

In a carcinogenicity study, groups of 50 male and 50 female F344 rats and B6C3F1 mice were given gavage doses of benzaldehyde (dissolved in corn oil) on 5 days/week for a period of 103 to 104 weeks. The doses given to the female mice were 300 and 600 mg/kg body weight per day, and to all

other groups 200 and 400 mg/kg body weight per day. Although tumors were found to form during the experiment, the increase in the incidence of some tumours in the male rats was not regarded as substance-related. An increase in the incidence of hyperplasia and squamous cell papillomas of the forestomach in mice were regarded as some evidence of carcinogenicity, but are probably the result of the irritative effects of benzaldehyde and are not of relevance because of the species-specific location (ECHA) [Kl. Score = 2].

Overall, therefore, there was no evidence in either mice or rats of a carcinogenic potential of benzaldehyde, which is in accordance with the, at most, low genotoxic activity of benzaldehyde in vitro.

I. Reproductive and Developmental Toxicity

Benzyl derivatives, including benzaldehyde, have been reported to produce no evidence of reproductive and developmental toxicity during various studies. It was also stated that as benzyl derivatives generally follow similar metabolic pathways, studies conducted on benzyl derivatives provide adequate evidence for benzaldehyde (ECHA).

In one available study 10 female rats were given oral doses of 2 mg benzaldehyde per animal (about 5 mg/kg body weight and day) every second day for a period of 223 days, and were mated with untreated males on days 75 and 108 after the beginning of treatment. The number of offspring. the weight of the pups after 1 and 3 weeks and survival of the pups was in the range of the control values. The number of pregnant females in the lest group was decreased relative to that in the control group (Sporn et al. 1967 as cited in ECHA). The study design (small number of treated animals, only one dose group) does not meet present-day standards and cannot, therefore, be regarded as evidence of impairment of female fertility (ECHA) [Kl. Score = 2].

The key study evaluating effects on fertility were by Kieckebusch and Lang (1960), which evaluated the effects of benzoic acid over 4 generations in rats via feeding. While this study does have some limitations, when supplemented by information on reproductive organs/tissues (sperm parameters, including epididymis/cauda epididimys/testis weights, sperm motility/density/abnormal sperm; Estrous cyclicity in females) from a 13 -week repeated dose study of benzyl acetate (a substances that is metabolized completely to benzoic acid) (Morrissey et al., 1988), the apparent gaps in data from the current OECD 443 study design are filled. Overall, taking into consideration both the Kieckebusch and Lang (1960), and Morrissey et al. (1988) studies, no effects on reproductive performance and off-spring were reported at 1% the test substance in feed (500 mg/kg bw). Therefore, the NOAEL for toxicity to reproduction is set at 500 mg/kg bw. (ECHA) [Kl. Score =2].

Sodium benzoate is the sodium salt of benzoic acid, and is completely metabolized to benzoic acid prior to excretion via the hippuric acid pathway. In a sub-acute developmental toxicity study conducted in rats and mice using sodium benzoate, dose levels applied showed no evidence of maternal toxicity. No effects on foetal development were reported. A NOAEL of 175 mg/kg bw/day was established. This level is considered to be very conservative and rats and mice seem to be the most sensitive species (ECHA) [Kl. Score = 2].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for benzaldehyde follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

The lowest NOAEL from these studies is 175 mg/kg-day based on absence of reproductive effects in a sub-acute developmental toxicity study in rats and mice. The NOAEL of 175 mg/kg-day will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 175/(10 x 10 x 1 x 10 x 1) = 175/1000 = 0.175 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.175 x 70 x 0.1)/2 = 0.61 mg/L

Cancer

There was no sufficient evidence of carcinogenicity in rat and mouse chronic studies conducted on benzaldehyde. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Benzaldehyde does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Benzaldehyde has moderate toxicity to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on benzaldehyde.

Table 3: Acute Aquatic Toxicity Studies on Benzaldehyde

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fathead minnow	96-hr LC_{50}	12.4	2	ECHA
Rainbow trout	96-hr LC_{50}	11.2	2	ECHA
Goldfish	96-hr LC_{50}	13.8	2	ECHA
Channel catfish	96-hr LC_{50}	5.39	2	ECHA
Bluegill	96-hr LC_{50}	1.07	2	ECHA
Daphnia magna	48-hr EC_{50}	19.7	1	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	33.1 (growth) 8.05 (yield)	1	ECHA

Chronic Studies

In a juvenile growth test, the 7-day NOEC to 1- day fathead minnow (*Pimephales promelas*) larvae was 0.12 mg/L (measured) based on growth rate and mortality (ECHA) [Kl. score = 2].

The 8-day NOEC to *Scenedesmus quadricauda* is 34 mg/L (ECHA) [Kl. score = 4].

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for benzaldehyde follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (1.07 mg/L), invertebrates (19.7 mg/L) and algae (8.05 mg/L0. Results from chronic studies are available for fish (0.12 mg/L) and algae (34 mg/L). On the basis that the data consists of short-term studies for three trophic levels and long-term results studies for two trophic levels, an assessment factor of 50 has been applied to the lowest reported NOEC of 0.12 mg/L for fish. The $PNEC_{water}$ is 0.002 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Moreover, the substance is not expected to substantially partition to sediments. Nonetheless, a $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.0016 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 1.0129/1280 \times 1000 \times 0.002$
$= 0.0016$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = 0.002 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 0.4436)/1000 \times 2400]$
$= 1.0129\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 11.09 \times 0.04$
$= 0.4436$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for benzaldehyde based on the molecular connectivity index (MCI) is 11.09 L/kg (EPA, 2019).
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.0003 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (0.22/1500) \times 1000 \times 0.002$
$= 0.0003$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 kg/m^3 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 11.09 \times 0.02$
$= 0.22\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for benzaldehyde based on the molecular connectivity index (MCI) is 11.09 L/kg (EPA, 2019).
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REAC Criteria methodology (DEWHA, 2009; ECHA, 2008).

Benzaldehyde is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 1.4, benzaldehyde does not meet the screening criteria for bioaccumulation.

The lowest chronic NOEC for benzaldehyde is >0.1 mg/L. The acute $E(L)C_{50}$ values are >1 mg/L. Thus, benzaldehyde does not meet the screening criteria for toxicity.

The overall conclusion is that benzaldehyde is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for benzaldehyde.

Attachment 2 Mass Balance Calculations

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Benzaldehyde	100-52-7	Not a PBT	No	No	No	No	No	No	2 (fish & algae) 1 (inv)	2 (fish) 1 (algae)	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern

DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
					0	30	0	30	0	30	
Benzaldehyde	100-52-7	3.60E+00	1.50E+01	4.80E-01	4.80E-02	1.20E-02	4.80E-04	1.20E-04	9.60E-06	2.40E-06	2.00E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

N-Benzyl-Alkylpyridium Chloride

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

N-benzyl-alkylpyridium chloride is a component in a water treatment product used to provide corrosion resistance from microbial influenced corrosion in the steel flowlines and spinelines throughout the produced water management collection system. Process and usage information for this chemical is summarised in **Table 1**.

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Percent Weight (%) in Product[1]
Benzyl-C-1-2-alkylpyridinium chloride	68909-18-2	Biocide	5

[1] Mid-point of range provided in SDS.
CAS No = Chemical Abstracts Service Number

The water treatment product could potentially be used for biocide treatment in FAPA but is currently not being used. Based on its use in other Santos project areas, dosage rates in water for this chemical in the biocide are in the range of 1.0×10^{-4} mg/L.

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. As detailed in the attachment and presented in **Table 2**, no data are available to derive toxicological reference and drinking water guideline values for n-benzyl-alkylpyridium chloride.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
N-benzyl-alkylpyridium chloride (68909-18-2)	- [a]	-	-	-	-	-

[a] – No data available.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** and the dossier regarding the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
N-benzyl-alkylpyridium chloride (68909-18-2)	Chronic *Daphnia* and algae	0.47	1000	0.0005

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
N-benzyl-alkylpyridium chloride (68909-18-2	[a]	-	-	0.078

[a]Calculated using equilibrium partitioning method.
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
N-benzyl-alkylpyridium chloride (68909-18-2	[a]	-	-	0.07

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

N-benzyl-alkylpyridium chloride is a mixture of alkyl pyridine quaternary ammonium salts. The molecular structure of n-benzyl-alkylpyridium chloride is presented in **Figure 1**. R1-5 are alkyl groups in the structure.

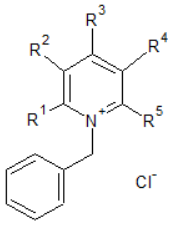

Figure 1 Molecular Structure of N-Benzyl-Alkylpyridium Chloride [2]

[2] Source https://echa.europa.eu/registration-dossier/-/registered-dossier/21246/1

N-benzyl-alkylpyridium chloride is inherently biodegradable. Components show variable sorption to soils and sediments. It is not expected to bioaccumulate based on the experimental octanol water partition coefficient (log K_{ow}).

The Persistent, Bioaccumulative and Toxic (PBT) assessment for n-benzyl-alkylpyridium chloride is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that n-benzyl-alkylpyridium chloride is not a PBT substance.

Human Health Hazards

There is a low concern for human health hazards. Very little information exists regarding the specific hazards associated with n-benzyl alkylpyridium chloride. Thus, the information provided in this assessment was taken from data collected for quaternary ammonium compounds in general. Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. As the substance is corrosive (i.e., pH=1.2), very little toxicity data are available with the exception of acute toxicity data showing a rat LD_{50} of approximately 50 mg/kg-day[3].

No data are available to derive toxicological reference and drinking water guideline values for n-benzyl-alkylpyridium chloride. Additional discussion is included in the dossier provided in **Attachment 1**.

Based on its potential use as a biocide in produced water flow lines, n-benzyl-alkylpyridium chloride may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to n-benzyl-alkylpyridium chloride in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay), and treatment and retention (and associated biodecay) are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of the biocide in produced water would be diluted by a factor of at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an

[3] LD50 = lethal dose of 50 percent of population; mg/kg bw – milligrams per kilogram body weight

'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. However, sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the sediment matrix.

PNECs for n-benzyl-alkylpyridium chloride are provided in **Tables 3-5**. Experimental toxicity data on water organisms was available for two trophic levels to calculate PNECs in water. There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, estimated Water Management Facility (WMF) pond influent concentrations (7.2×10^{-10} mg/L, refer **Attachment 2**) are well less than PNECs for aquatic receptors (5×10^{-3} mg/L). Blending within the storage pond, degradation during storage and treatment would further reduce concentrations.

References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019..

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Attachment 1 Risk Assessment Dossier

N-benzyl-alkylpyridium chloride

This dossier on N-benzyl-alkylpyridium chloride presents the most critical studies pertinent to the risk assessment of this substance in its use in drilling muds, hydraulic fracturing fluids and water treatment systems. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from The National Industrial Chemicals Notification and Assessment Scheme (NICNAS, 1994) and the ECHA database that provides information on chemicals that have been registered under the European Union (EU) REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – N-benzyl-alkylpyridium chloride was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. N-benzyl-alkylpyridium chloride was assessed as a tier 2 chemical for acute toxicity and chronic toxicity. Therefore, N-benzyl-alkylpyridium chloride is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

N-benzyl-alkylpyridium chloride is a mixture of alkyl pyridine quaternary ammonium salts. The substance is inherently biodegradable. Components show variable sorption to soils and sediments. It is not expected to bioaccumulate based on the experimental octanol water partition coefficient (log K_{ow}). Very little information exists regarding the specific human health hazards associated with N-benzyl alkylpyridium chloride. Thus, the information provided in this dossier is taken from data collected for quaternary ammonium compounds in general. Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. As the substance is corrosive (i.e., pH=1.2), very little toxicity data are available with the exception of acute toxicity data which indicates a low concern for human health hazards. In regard to environmental hazard, N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. However, sediment dwelling organisms are far less sensitive to the substance based on combined effects of biodegradation and binding to the settlement matrix.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1-benzyl-1-methyl-2H-pyridin-1-ium; chloride
CAS RN: 68909-18-2
Molecular formula: $C_{12}H_7ClNR1R2R3R4R5$, where R1-5 are alkyl groups
Molecular weight: 221.72 g/mol

Synonyms: Pyridinium, 1-(phenylmethyl)-, Et Me derivs., chlorides, Pyridinium, methyl-1-(phenylmethyl)-, chloride, N-Benzylpicolinonium chloride, Pyridinium, methyl-1-(phenylmethyl)-, chloride (1:1)

3 PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of Physico-Chemical Properties of on N-benzyl-alkylpyridium chloride.

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	Liquid	1	ECHA
Melting Point	-57.27 °C @ 101.3 kPa	1	ECHA
Boiling Point	116.34 °C @ 101.3 kPa	1	ECHA
Density	1,104 kg/m^3	1	ECHA
Vapour Pressure	200 Pa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	3 @ 25°C	2	ECHA
Water Solubility	100 g/L @ 30°C	1	ECHA
Viscosity	47.9 mm^2/s (static) @ 38°C	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for N-benzyl-alkylpyridium chloride.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

N-benzyl-alkylpyridium chloride is inherently biodegradable. Components show variable sorption to soils and sediments. It is not expected to bioaccumulate based on the experimental log K_{ow}.

N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance based on combined effects of biodegradation and binding to the settlement matrix.

B. Biodegradation

The ready biodegradation of N-benzyl-alkylpyridium chloride in seawater was determined according to OCED guideline 306 (Biodegradability in Seawater). The rate of degradation was estimated at 13% in seawater assay. The substance was considered likely to be inherently biodegradable (ECHA) [Kl Score=3].

C. Environmental Distribution

Adsorption/desorption

A screening test conducted in accordance with OECD 121 indicated that due to its multi component nature, N-benzyl-alkylpyridium chloride displayed a range of Log K_{oc} values from <1.25 to 5.40. The substance is considered to be a UVCB substance comprising multiple components, of similar chemical functionality, in varying proportions. A quantitative assessment of these components would therefore present considerable technical difficulty as there is not considered to be an analytical method that is sufficiently sensitive, and so a more detailed assessment in accordance with OECD 106 for example would not be technically possible. For the purposes of this dossier, a log K_{oc} is estimated to be a midpoint of the range stated above (i.e., approximately 3).

D. Bioaccumulation

No bioconcentration studies have been conducted on N-benzyl alkylpyridium chloride. N-benzyl alkylpyridium chloride is not expected to bioaccumulate based on the experimental log K_{ow} of 3 (ECHA) [Kl. score = 1].

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Very little information exists regarding the specific hazards associated with N-benzyl alkylpyridium chloride. Thus, the information provided in this section is taken from data collected for quaternary ammonium compounds in general.

Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. As the substance is corrosive (i.e., pH=1.2), very little toxicity data are available with the exception of acute toxicity data showing a rat LD_{50} of approximately 50 mg/kg-day.

B. Toxicokinetics

No toxicokinetic data are available for these substances, however the data on related quaternary ammonium compounds are summarised below.

Absorption

Significant absorption of quaternary ammonium compounds is unlikely due to their highly ionic nature. WHO (1998) reports the oral absorption of quaternary ammonium compounds in general to be poor. A published Canadian review of the toxicity of the quaternary ammonium compound didecyldimethylammonium chloride (DDAC) notes experiments in rats in which up to 99% of orally administered radioactivity was recovered in the faeces and less than 2.5% in the urine (ECHA 2020). .

The dermal absorption of quaternary ammonium compounds is likely to be low based on the chemical structure, ionic nature, molecular weight and lack of lipophilicity of the substance. Absorption of this group of substances through skin is also indicated to be very low based on an absence of reports of systemic effects following dermal exposure (WHO, 1998). However, it is noted that the substance is corrosive, therefore it is possible that systemic absorption may occur following significant accidental dermal exposures resulting in skin burns, where the normal barrier integrity of the skin is compromised. Buist et al (2007) reported very low dermal penetration (0.5%) for the quaternary ammonium compound DDAC in human skin in vitro over a 48-hour period.

No data are available for absorption following inhalation exposure; however, it is considered unlikely that absorption by his route of exposure would be significant. Although not relevant to the human risk assessment, the WHO document notes that the systemic absorption of quaternary ammonium compounds following parenteral administration is 'possible'.

Distribution

No data on distribution are available. However, given the water solubility of the substance, it is likely to be widely distributed via the circulation if absorbed.

Metabolism

No data are available for the substance; however significant metabolism is not predicted given the likely poor systemic absorption. A published Canadian review of the toxicity of the quaternary ammonium compound DDAC reports some oxidative metabolism of the decyl sidechain, but no molecular cleavage by N-dealkylation (Henderson, 1992).

Excretion

Data indicate that quaternary ammonium compounds are largely excreted in the faeces (WHO, 1998; Henderson, 1992). The poor absorption and chemical nature of the substance (specifically the lack of lipophilicity) indicate that substance quaternary ammonium compounds have no or little potential for bioaccumulation.

C. Acute Toxicity

The oral LD_{50} in rats is 50.1 milligrams per kilogram (mg/kg, HPVIS) [Kl. score = 2]. There are no acute inhalation or dermal toxicity studies on N-benzyl-alkylpyridium chloride.

D. Irritation

No studies are available. However, N-benzyl-alkylpyridium chloride is considered corrosive based on its pH of 1.2 (ECHA).

E. Sensitisation

No studies are available.

F. Repeated Dose Toxicity

No studies are available.

G. Genotoxicity

The *in vitro* genotoxicity studies on N-benzyl-alkylpyridium chloride are presented in Table 3.

Table 3 In vitro Genotoxicity Studies on N-benzyl-alkylpyridium chloride

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains	-	-	1	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	ECHA
Chromosomal aberrations (human lymphocytes)	-	-	1	ECHA

*+, positive; -, negative

H. Carcinogenicity

No studies are available.

I. Reproductive Toxicity

No studies are available.

J. Developmental Toxicity

No studies are available.

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

No data are available on N-benzyl-alkylpyridium chloride to derive oral toxicological reference and drinking water guidance values.

L. Human Health Hazard Assessment Of Physico-Chemical Properties

N-benzyl-alkylpyridium chloride does not exhibit the following physico-chemical properties:

- Explosivity
- Oxidising potential

The substance is classified as flammable (Flam. Liquid 3).

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

N-benzyl-alkylpyridium chloride exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the sediment matrix.

B. Aquatic Toxicity

Table 4 lists the results of acute aquatic toxicity studies on salts of N-benzyl-alkylpyridium chloride.

Table 4 Acute Aquatic Toxicity Studies on N-benzylalkylpyridium chloride

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Cyprinodon variegatus	96-hr LC_{50}	14.1	1	ECHA
Daphnia magna	48-hr EC_{50}	3.1	1	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	0.47	1	ECHA

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

PNEC water

Experimental results are available for two trophic levels. Acute EC_{50} values are available for *Daphnia* (3.1 milligrams per litre [mg/L]), and algae (0.47 mg/L). On the basis that the data consists of short-term results from two trophic levels, an assessment factor of 1,000 has been applied to the lowest reported $E(L)C_{50}$ value of 0.47 mg/L for algae. The $PNEC_{water}$ is 0.0005 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.078 mg/kg wet weight.
The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (20/1280) \times 1000 \times 0.0025$
$= 0.078$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = 0.005 mg/L

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 4.8)/1000 \times 2400]$
$= 3.1\ m^3/m^3$

Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

And:
$Kp_{sed} = K_{oc} \times f_{oc}$
= 1000 x 0.04
= 40 L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for sediment is 1000.
f_{oc} = fraction of organic carbon suspended sediment = 0.04 [default].

PNEC soil

There are no EC_{10} or NOEC values for terrestrial receptors. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.07 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
= (20/1500) x 1000 x 0.0013
= 0.07 mg/kg soil dry weight

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = 0.005 mg/L

$Kp_{soil} = K_{oc} \times f_{oc}$
= 1000 x 0.02
= 20 m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} was estimated to be 1000 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

N-benzyl alkylpyridium chloride is estimated to be ultimately biodegradable.

No bioconcentration studies are available for N-benzyl alkylpyridium chloride. However. the measured log K_{ow} for N-benzyl alkylpyridium chloride is 3; thus, N-benzyl alkylpyridium chloride does not meet the screening criteria for bioaccumulation.

The acute EC_{50} values for N-benzyl alkylpyridium chloride in algae is <1 mg/L. Thus, N-benzyl alkylpyridium chloride meets the screening criteria for toxicity.

The overall conclusion is that N-benzyl alkylpyridium chloride is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for N-benzyl-alkylpyridium.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
N-benzyl-alkylpyridium chloride	68909-18-2	Not a PBT	No	No	No	No	No	Yes	2	No Data	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor

COC	constituent of concern
DDAC	didecyldimethylammonium chloride
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LD	lethal dose
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mm^2/s	square millimetre per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

WHO	World Health Organization

Attachment 2 Contingency Biocide Dosing Assumptions

Attachment 2
Summary of Exposure Point Concentration Development
(Contingency Water Treatment Chemicals)

Mass Balance

In other Santos project areas, approximately 413 milligrams per litre (mg/L) of a water treatment product is being dosed (9.2 litres [L] added to approximately 1,380 billion barrels [bbl] or 2.2 x 10^5 litres of legacy/CF1 PFW). The constituent of potential concern (COPC) legacy/CF1 produced formation water (PFW) concentrations are calculated based on the product dose that is apportioned between the COPCs based on the COPC percent weight in the product (composition information in the safety data sheet). The concentration of the COPCs in the water storage pond influent (representative of treatment of combined produced water from legacy/CF1 PFW and bore water) was based on the combined dilution from 2,300 bbl/day.

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	COPC Legacy/CF1 PFW (mg/L)	Storage Pond Influent (mg/L)
Benzyl-C1-2-alkylpyridinium chloride	68909-18-2	5	1.0E-04	7.2E-10

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
mg/L = milligrams per litre
PFW = produced formation water

Qualitative Tier 2 Assessment

Boric Acid and Sodium Tetraborate Decahydrate (Borax)

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for these Tier 2 chemicals includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Boric acid and borax are components in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for these chemicals in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Boric Acid	10043-35-3	Crosslinker	<0.1%
Sodium Tetraborate Decahydrate (Borax)	1303-96-4	Crosslinker	<0.01 %

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

In the environment, borates and compounds of boric acid will dissociate and/or hydrolyse to form the same boron species. As a result, boric acid and borax have been assessed together in this assessment as a group. The assessment of toxicity of these chemicals was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. Boric acid and borax are boron compounds. Since an Australian Drinking Water Guideline (ADWG) Value is available for boron (see **Table 2**), toxicological reference values (TRVs) were not derived for

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

these chemicals. A detailed discussion of the drinking water guideline values is presented in **Attachment 1**.

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Boric Acid (CAS No. 10043-35-3) Borax (CAS No. 1303-96-4	Boron	4 mg/L

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNEC for soil is detailed in **Table 4**. PNECs for sediment were not calculated. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Boric Acid (CAS No. 10043-35-3) Borax (CAS No. 1303-96-4	-	-	-	0.94[a]

$PNEC_{water}$ for boric acid and borax is the ANZG Water Quality Guideline – Freshwater Trigger Value for boron.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Boric Acid (CAS No. 10043-35-3) Borax (CAS No. 1303-96-4	[a]	-	-	5.7

[a] Calculated using species sensitivity distribution method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by these Tier 2 chemicals is provided in the following sections.

General Overview

Boric acid and borax are boron compounds. Boron is almost exclusively found in the environment in the form of boron-oxygen compounds, which are often referred to as borates. The high strength of the B-O bond relative to those between boron and other elements makes boron oxide compounds stable compared to nearly all non-oxide boron materials.

The molecular structure for boric acid is presented in **Figure 1**. The molecular structure for borax is presented in **Figure 2**.

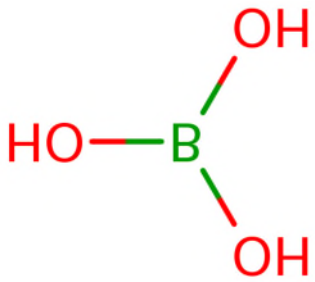

Figure 1 Molecular Structure of Boric Acid[2]

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/10043-35-3

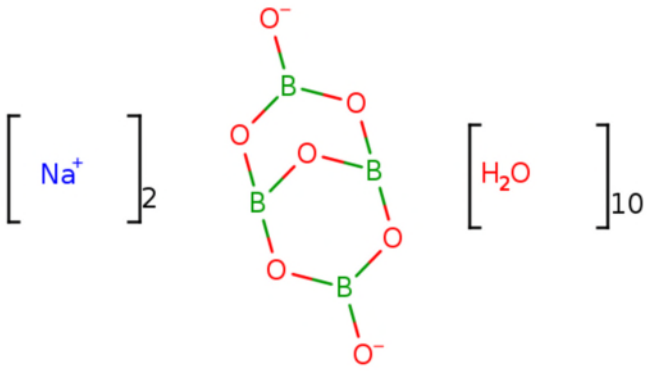

Figure 2 Molecular Structure of Borax[3]

In the environment, borates and compounds of boric acid will dissociate and/or hydrolyse to form the same boron species. For example, when borax dissolves in dilute solutions, it dissociates into Na^+ ions and the tetraborate anion ($B_4O_5(OH)_4^{2-}$). Boric acid ($B(OH)_3$) is formed following acid catalysed hydrolysis of the tetraborate anion. Under alkaline conditions, dilute solutions of the tetraborate anion depolymerise rapidly to the mononuclear borate anion ($B(OH)_4^-$) (NICNAS, 2019).

Borax will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Degradation is not applicable to inorganic borates. Boric acid is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for boric acid and borax is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substances are not a PBT substance.

Human Health Hazards

Borax exhibits low acute toxicity by the oral and dermal routes. Boric acid exhibits low acute toxicity by the oral, dermal and inhalation routes. Neither substance is a skin or eye irritant, nor a skin sensitizer.

In aqueous media at physiological pH, borax will predominantly exist as un-dissociated boric acid. The developing fetus and the testes are the two most sensitive targets of boron toxicity in multiple species. The testicular effects include reduced organ weight and organ to body weight ratio, atrophy, degeneration of the spermatogenic epithelium, impaired spermatogenesis, reduced fertility, and sterility. The developmental effects from boron exposure include high prenatal mortality; reduced fetal body weight; and malformations and variations. Repeated inhalation exposure to read-across substance boron oxide resulted in slight irritation to the respiratory tract, but no systemic toxicity. Boric acid was not genotoxic; and boric acid and borax was not carcinogenic to rodents.

[3] Source https://chem.nlm.nih.gov/chemidplus/rn/1303-96-4

TRVs were not derived for boric acid or borax. The health-based ADWG value for boron is 4 milligrams per litre (mg/L) (see **Table 2**). A detailed discussion of the drinking water guideline values is presented in **Attachment 1**.

Boric acid or borax (as boron) may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to boric acid or borax in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, boric acid and borax has low acute and chronic toxicity to aquatic organisms.

Borax will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions. Boric acid is highly water soluble and it tends to remain in surface waters. Although some partitioning from water to soil and sediment does occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5 to9.0) (NICNAS, 2019).

ANZG derived a freshwater high reliability trigger value for boron of 940 µg/L using the statistical distribution method at 95% protection (ANZG, 2021). The 95% species protection level for boron in freshwater (940 µg/L) is recommended for adoption in the assessment of slightly-to-moderately disturbed ecosystems. Considering the land uses adjacent to the Dawson River include light to moderate grazing, and there is some development upstream of the Horseshoe Lakes, adoption of the 95% species protection criteria is considered appropriate (AECOM, 2019).

Limited sediment toxicity data are available for boric acid and boron containing compounds in general (NICNAS, 2019). Due to the high water solubility of boron and its low partitioning to sediment, sediment toxicity testing for boron is particularly challenging as it is difficult to ensure that exposure is through the solid phase (i.e., sediment) and not from the aqueous boric acid in the overlying water (NICNAS, 2019). Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics. Therefore, a PNEC for sediment could not be calculated using the equilibrium partitioning method. As a result, the assessment of this compartment will be covered by the aquatic assessment.

A PNEC for soil was calculated for boron using the species sensitivity distribution method (see **Table 3**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, in accordance with EA conditions, managed release of treated water to the Dawson River is monitored for boron.

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Attachment 1 Risk Assessment Dossier

BORIC ACID (CAS No. 10043-35-3)

SODIUM TETRABORATE DECAHYDRATE (BORAX) (CAS No. 1303-96-4)

This dossier presents the most critical studies pertinent to the risk assessment of two boron compounds (boric acid and borax) in their use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Borax and boric acid were assessed as tier 1 chemicals for acute and chronic aquatic toxicity. Neither is a PBT substance. However, both substances were identified in chemical databases used by NICNAS as an indicator that the chemicals are of concern. Therefore, these substances are classified overall as **tier 2** chemicals and require a hazard assessment and qualitative assessment of risk.

1. BACKGROUND

Boric acid and borax are boron compounds. As boron is an essential plant nutrient, soluble boron compounds (including borax) have an agricultural application as fertilisers in boron deficient soils, with these compounds being applied directly to soil or as a foliar spray (NSW Agriculture, 2003). Boron compounds, including boric acid, are used in domestic coal seam gas (CSG) applications (Commonwealth of Australia, 2014).

Borax will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Degradation is not applicable to inorganic borates. Boric acid is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation. Borax and boric acid have low acute and chronic toxicity to aquatic organisms.

Borax exhibits low acute toxicity by the oral and dermal routes. Boric acid exhibits low acute toxicity by the oral, dermal and inhalation routes. Neither substance is a skin or eye irritant, nor a skin sensitizer. In aqueous media at physiological pH, borax will predominantly exist as un-dissociated boric acid. The developing fetus and the testes are the two most sensitive targets of boron toxicity in multiple species. The testicular effects include reduced organ weight and organ to body weight ratio, atrophy, degeneration of the spermatogenic epithelium, impaired spermatogenesis, reduced fertility, and sterility. The developmental effects from boron exposure include high prenatal mortality; reduced fetal body weight; and malformations and variations. Repeated inhalation exposure to read-across substance boron oxide resulted in slight irritation to the respiratory tract, but no systemic toxicity. Boric acid was not genotoxic; and, boric acid and borax was not carcinogenic to rodents.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): boric acid

CAS RN: 10043-35-3

Molecular formula: BH_3O_3

Molecular weight: 61.84 g/mol

Synonyms: orthoboric acid; boracic acid; borofax; boron hydroxide; boron trihydroxide

Chemical Name (IUPAC): disodium bicyclo[3.3.1]tetraboroxane-3,7-bis(olate)

CAS RN: 1303-96-4

Molecular formula: $B_4Na_2O_7$

Molecular weight: 381.4 g/mol

Synonyms: sodium tetraborate decahydrate; borax; monosodium metaborate; sodium borate; sodium borate (NaBO2); sodium diborate; sodium meta borate; sodium metaborate; sodium tetraborate

3. PHYSICAL AND CHEMICAL PROPERTIES

Limited measured data are available for borax. In the environment, borax is expected to dissociate and/or hydrolyse to release boric acid at neutral pH. Therefore, measured data available for boric acid have been presented as analogue data for this substance.

Key physical and chemical properties for boric acid are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Boric Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, odorless, crystalline solid	2	ECHA
Melting Point	>100°C (decomposes)	1	ECHA
Boiling Point	Not Applicable	-	ECHA
Density	1489 kg/m^3 @ 20°C	1	ECHA
Vapor Pressure	0 Pa @ 25°C	1	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	Not Applicable, substance is inorganic	-	ECHA
Water Solubility	48.8 g/L @ 20°C	1	ECHA
Dissociation Constant (pKa)	8.94 @ 20°C	1	ECHA

Boron is almost exclusively found in the environment in the form of boron-oxygen compounds, which are often referred to as borates. The high strength of the B-O bond relative to those between boron and other elements makes boron oxide compounds stable compared to nearly all non-oxide boron materials. Indeed, the B-O bond is among the strongest found in the chemistry of naturally occurring inorganic substances (ECHA).

In the environment, borates and compounds of boric acid will dissociate and/or hydrolyse to form the same boron species. For example, when borax dissolves in dilute solutions, it dissociates into Na^+ ions and the tetraborate anion ($B_4O_5(OH)_4^{2-}$). Boric acid ($B(OH)_3$) is formed following acid catalysed hydrolysis of the tetraborate anion. Under alkaline conditions, dilute solutions of the tetraborate anion depolymerise rapidly to the mononuclear borate anion ($B(OH)_4^-$) (NICNAS, 2019).

Boric acid is a Lewis acid that acts as a weak monoprotic acid by accepting OH^- and not as a proton donor (pKa 9.14). Therefore, at the near neutral pH of most environmental systems and at low concentrations (<0.025 mol B/L), the neutral mononuclear species ($B(OH)_3$) will dominate and only a small proportion of boron will exist as the borate monoanion, $B(OH)_4^-$. Therefore, in the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions (NICNAS, 2019).

Exposure to borates are often expressed in terms of boron (B) equivalents based on the fraction of boron in the source substance on a molecular weight basis. The B equivalents used are a generic designation rather than a designation of the element boron. The factor for converting boric acid to B-equivalents is 0.1748. The factor for converting borax to B-equivalents is 0.2149.

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for boric acid or borax.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	See Below

Convention, Protocol or other international control	Listed Yes or No?
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

Boric acid and borax have both been identified as a Substance of Very High Concern and recommended for inclusion in Annex XIV (the Authorisation List) of the REACH legislation in the European Union on the basis of its toxicity for reproduction (Article 57c). The chemicals are on the "Candidate List" and are not on the "Authorisation List". The chemicals are not currently identified as being of environmental concern (NICNAS, 2019).

5. ENVIRONMENTAL FATE PROPERTIES

A. Summary

Borax will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Degradation is not applicable to inorganic borates. Boric acid is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

B. Partitioning

Borax will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions. Boric acid is highly water soluble and it tends to remain in surface waters. Although some partitioning from water to soil and sediment does occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5 to 9.0) (NICNAS, 2019).

C. Biodegradation

Degradation is not applicable to inorganic borates. It is not subject to hydrolysis, photodegradation, or biodegradation (ECHA). Inorganic borates are subject to chemical transformation processes (adsorption, complexation, precipitation, fixation) once released into the environment (ECHA).

D. Environmental Distribution

The Kp value for boron compounds was calculated as the median of all measured Kp values from the GEMAS project (Geochemical Mapping of Agricultural and Grazing Land Soil project): 2.19 L/kg dry weight (ECHA) [Kl. Score = 2]. The chemistry of boron in soils and aquatic systems is simplified by the absence of oxidation- reduction reactions or volatilization. Redox processes can mobilize Fe oxides and Mn oxides, which may lead to a release of boron in aquatic systems. Generally, sediments are characterised with higher pH values than the soil matrix, which increases the boron sorption capacity (ECHA).

If released to soil, based on this low Kp value, low vapour pressure and high water solubility, boric acid and borax are considered relatively mobile in the environment, under certain conditions (ECHA).

E. Bioaccumulation

The WHO review of boron (WHO, 1998) noted that "highly water soluble materials are unlikely to bioaccumulate to any significant degree and that borate species are all present essentially as un-dissociated and highly soluble boric acid at neutral pH". BCFs of <0.1 to 10.5 L/kg have been reported from laboratory tests of fish and oysters (Hamilton and Wiedmeyer, 1990; Thompson et al. 1976).

6. HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Borax exhibits low acute toxicity by the oral and dermal routes. Boric acid exhibits low acute toxicity by the oral, dermal and inhalation routes. Neither substance is a skin or eye irritant, nor a skin sensitizer. In aqueous media at physiological pH, borax will predominantly exist as un-dissociated boric acid. The developing fetus and the testes are the two most sensitive targets of boron toxicity in multiple species. The testicular effects include reduced organ weight and organ to body weight ratio, atrophy, degeneration of the spermatogenic epithelium, impaired spermatogenesis, reduced fertility, and sterility. The developmental effects from boron exposure include high prenatal mortality; reduced fetal body weight; and malformations and variations. Repeated inhalation exposure to read-across substance boron oxide resulted in slight irritation to the respiratory tract, but no systemic toxicity. Boric acid was not genotoxic; and boric acid and borax was not carcinogenic to rodents.

B. Toxicokinetics

Boric acid is not metabolised in either animals or humans, owing to the high energy level required (523 kJ/mol) to break the B - O bond. Other inorganic borates convert to boric acid at physiological pH in the aqueous layer overlying the mucosal surfaces prior to absorption. Most of the simple inorganic borates exist predominantly as undissociated boric acid in dilute aqueous solution at physiological and environmental pH, leading to the conclusion that the main species in the plasma of mammals is un-dissociated boric acid. Since other borates dissociate to form boric acid in aqueous solutions, they too can be considered to exist as un-dissociated boric acid under the same conditions. Additional support for this derives from studies in which more than 90 % of administered doses of inorganic borates are excreted in the urine as boric acid. Absorption of borates via the oral route is nearly 100 %. For the inhalation route also 100 % absorption is assumed as worst case scenario. Dermal absorption through intact skin is very low with a percent dose absorbed of 0.226 ± 0.125 in humans. Using the % dose absorbed plus standard deviation (SD) for boric acid, a dermal absorption for borates of 0.5 % (rounded from 0.45 %) can be assumed as a worse case estimate (ECHA).

In the blood boric acid is the main species present and is not further metabolised. Boric acid is distributed rapidly and evenly through the body, with concentrations in bone 2 - 3 higher than in other tissues. Boric acid is excreted rapidly, with elimination half-lives of 1 hour in the mouse, 3 hours in the rat and < 27.8 hours in humans, and has low potential for accumulation. Boric acid is mainly excreted in the urine (ECHA).

C. Acute Toxicity

The oral LD_{50} of borax in rats is > 2,500 mg/kg (ECHA) [Kl. score = 1]. The oral LD_{50} of boric acid in rats is 3,450 mg/kg (ECHA) [Kl. score = 1].

There are no acute inhalation studies on borax. In a read-across study for borax, the 4-hour inhalation LC_{50} value for disodium tetraborate pentahydrate in rats is >2.04 mg/L (ECHA) [Kl. score = 1]. The 4-hour inhalation LC_{50} value for boric acid in rats is >2.01 mg/L. The mass median aerodynamic diameter (MMAD) was 2.8 µm (ECHA) [Kl. score = 1]. In another study, the 4-hour inhalation LC_{50} value for boric acid in rats was >2.03 mg/L (ECHA) [Kl. score = 1].

The dermal LD_{50} of borax in rabbits is >2,000 mg/kg (ECHA) [Kl. score = 2]. The dermal LD_{50} of boric acid in rabbits is >2,000 mg/kg (ECHA) [Kl. score = 1].

D. Irritation

Application of 0.5 g. of borax to the skin of rabbits for 4 hours under occlusive conditions was not irritating. The mean erythema and edema scores were 0.00 (ECHA) [Kl. scores = 2]. Application of 0.5 g. of boric acid to the skin of rabbits for 24 hours under occlusive conditions was not irritating. The mean of the 24 and 72 hour scores were: 0.13 for erythema and 0.00 for edema (ECHA) [Kl. scores = 1].

Disodium tetraborates are eye irritants. Instillation of 0.08 mL of read-across substance disodium tetraborate pentahydrate into the eyes of rabbits was slightly irritating. The mean of 24, 48, and 72 hours scores were: 0.22 for corneal opacity; 0.22 for iridial lesions; 2.8 for conjunctival redness; and 1.89 for chemosis. The effects were fully reversible (ECHA) [Kl. score = 1].

Boric acid induced mild conjunctivae redness and chemosis and minor effects on the iris. The effects were reversible within 7 days (ECHA). Instillation of 100 mg of boric acid into the eyes of rabbits was slightly irritating. The mean of 24, 48, and 72 hours scores were: 0.00 for corneal opacity; 0.11 for iridial lesions; 0.94 for conjunctival redness; and 0.56 for chemosis (ECHA) [Kl. score = 1].

E. Sensitization

There are no skin sensitization studies on Borax. Read-across substances disodium tetraborate pentahydrate was not a skin sensitizer to guinea pigs in a Buehler test (ECHA) [Kl. score = 1].

Boric acid was not a skin sensitizer to guinea pigs in a Buehler test (ECHA) [Kl. score = 1]. Sodium tetraborate pentahydrate was not a skin sensitizer to guinea pigs in a Buehler test (ECHA) [Kl. score = 1]. Sodium tetraborate decahydrate was not a skin sensitizer to guinea pigs in a Buehler test (ECHA) [Kl. score = 1].

F. Repeated Dose Toxicity

Oral

Male and female SD rats were given in their feed boric acid at doses of 0, 52.5, 175, 525, 1,750 or 5,250 ppm B equivalents for 90 days. The average intake has been estimated to be approximately 0, 2.6, 8.8, 26, 87.5 or 262.5 mg B/kg-day, respectively (EPA, 2004). By week 6, all of the animals in the

highest dose died. Clinical signs in the top two dose levels were rapid respiration, inflamed eyes, swollen paws, and desquamated skin on the paws and tails. There was also reduced food consumption and body weight gain. The 1,750 ppm females showed reduced liver, spleen ovary, and adrenal weights; the 1,750 ppm males showed reduced liver, spleen, kidney, testes, and adrenal weights. The adrenals of 4 of the 1,750 ppm males showed minor increases in lipid content and size of the cells in the zona reticularis. Atropied testis (complete atrophy of the spermatogenic epithelium and decreased in the size of the seminiferous tubules) was seen in all of the 1,750 ppm males. One 525 ppm male had partial testicular atrophy. The NOAEL for this study is 175 ppm boron or 8.8 mg B/kg-day (Weir and Fisher, 1972). [Kl. score = 2]

Male and female SD rats were given in their diet borax at doses of 0, 52.5, 175, 525, 1,750 or 5,250 ppm B equivalents for 90 days. The average intake has been estimated to be approximately 0, 2.6, 8.8, 26, 87.5 or 262.5 mg B/kg-day, respectively (EPA, 2004). By week 6, all of the animals in the highest dose died. Clinical signs in the top two dose levels were rapid respiration, inflamed eyes, swollen paws, and desquamated skin on the paws and tails. There was also reduced food consumption and body weight gain. The 1,750 ppm females showed reduced liver, spleen and ovary weights; the 1,750 ppm males showed reduced liver, spleen, kidney, testes, and brain weights. The adrenals of the majority of the 1,750 ppm males and females showed slight to moderate increases in lipid content and size of the cells in the zona reticularis. Atropied testis (complete atrophy of the spermatogenic epithelium and decreased in the size of the seminiferous tubules) was seen in all of the 1,750 ppm males. Four 525 ppm males had partial testicular atrophy. Spermatogenic arrest was found in one 525 ppm male. The NOAEL for this study is 175 ppm boron or 8.8 mg B/kg-day (Weir and Fisher, 1972). [Kl. score = 2]

Male and female B6CF1_1 mice were given in the diet 0, 1,200, 2,500, 5,000, 10,000 or 20,000 ppm boric acid for 13 weeks (control and highest dose group) or 16 weeks (remaining dose groups). These dietary levels correspond to approximately 0, 34, 70, 141, 281 and 563 mg B/kg-day for males, respectively; and 0, 47, 97, 194, 388 and 776 mg B/kg-day for females, respectively (EPA, 2004). There was mortality (8/10 males; 6/10, females) in the 20,000 ppm, as well as hyperkeratosis and acanthosis. One male also died in 10,000 ppm group. Degeneration or atrophy of the seminiferous tubules occurred in the $\geq$5,000 ppm males. Minimal to mild extramedullary hematopoiesis of the spleen was observed in all dose groups. The LOAEL for this study is 1,200 ppm, corresponding to 34 and 47 mg B/kg-day for males and females, respectively (NTP 1987). [Kl. score = 2]

Male and female SD rats were given in their diet 0, 117, 350 or 1,170 ppm boric acid for two years. The average intake has been estimated to be approximately 0, 5.9, 17.5 or 58.5 mg B/kg-day, respectively (EPA, 2004). The 1,170 ppm rats had decreased food consumption during the first 13 weeks of the study and suppressed growth throughout the study. Signs of toxicity in the 1,170 ppm animals included swelling and desquamation of the paws, scaly tails, inflammation of the eyelids, and bloody discharge from the eyes. All of the 1,170 ppm males had testicular atrophy at the 6, 12 and 24 month time points. The seminiferous epithelium was atrophied, and the tubular size in the testes was decreased. There were significant decreases in the absolute and relative testes weights. Brain and relative thyroid weights were increased. The NOAEL for this study is 350 ppm B equivalents or 17.5 mg B/kg-day (Weir and Fisher, 1972). [Kl. score = 2]

Male and female B6C3F$_1$ mice were given up to 20,000 ppm boric acid in their feed for 13 weeks (NTP, 1987). Eight out of the ten males and six out of the ten females from the 20,000 ppm group died and one of the ten males from the 10,000 ppm group died before end of study. Symptoms included nervousness, haunched appearance, dehydration, foot lesions and scaly tails. Incidences of

extra medullary heamatopoiesis of spleen observed of varying severity in all dose groups for both males and females and hyperkeratosis and/or acanthosis of the stomach observed at the highest dose only in both males and females. At doses > 5,000 ppm (142 mg B/kg bw for the male), degeneration or atrophy of the seminiferous tubules was observed. The NOAEL for this study is 34 mg B/kg-day (NTP, 1987). [Kl. score = 2]

Inhalation

Male and female rats were exposed by inhalation to 0, 77, 175, or 470 mg/m^3 boron oxide. The exposures were 6 hours/day, 5 days/week for 24, 12, and 10 weeks for the 77, 175, and 470 mg/m^3 concentrations groups, respectively. The MMAD were 2.5, 1.9, and 2.4 µm for the 77, 175, and 479 mg/m^3 concentrations groups, respectively. There was no evidence of systemic toxicity. Some of the 470 mg/m^3 had reddish exudate from the nose. As these animals were covered with dust, this effect may have been local irritation of the nose and from the animals scratching the nose. The NOAEL for systemic toxicity is 470 mg/m^3, the highest exposure concentration tested. The NOAEL for localized effects (irritation) is 175 mg/m^3 (ECHA). [Kl. score = 2]

Dermal

No studies are available.

G. Genotoxicity

In Vitro Studies

There are no *in vitro* genotoxicity studies on borax. Table 3 presents the results of the *in vitro* genotoxicity studies on boric acid.

Table 3: *In vitro* Genotoxicity Studies on Boric Acid

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	1	ECHA
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	2	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	ECHA
Chromosomal aberrations (Chinese Hamster Ovary cells)	-	-	1	ECHA
Chromosomal aberrations (Chinese Hamster Ovary cells)	-	-	1	ECHA
Chromosomal aberrations (Human peripheral lymphocytes)	NS	+	2	ECHA
Unscheduled DNA synthesis (rat liver cells)	NA	-	1	ECHA

*+, positive; -, negative; NA, not applicable; NS, not specified.

In Vivo Studies

No studies are available on borax.

Male and female Swiss Webster mice were given two daily doses of 0, 225, 450, 900, 1,800, or 3,500 mg/kg boric acid. The frequency of micronucleated polychromatic erythrocytes were not increased at any dose level (ECHA) [Kl. score = 1].

H. Carcinogenicity

Oral

Male and female SD rats were given in their diet disodium tetraborate decahydrate (Borax) or boric acid at doses of 0, 117, 350, or 1,170 ppm as B equivalents (approximately 0, 5.9, 17.5, or 58.5 mg B/kg-day) for two years. There was no mention of tumors in the report. Nevertheless, NTP (1987) concluded that this study provided adequate data on the lack of carcinogenic effects of boric acid in rats (Weir and Fisher, 1972; EPA, 2004).

Male and female B6C3F_1 mice were given in their diet 0, 2,500, or 5,000 ppm boric acid for 103 weeks. The dietary levels are equivalent to 0, 446, or 1,150 mg/kg-day boric acid or 0, 78.1, or 201.3 mg B/kg-day. There was no evidence of carcinogenicity (NTP, 1987). [Kl. score = 2]

I. Reproductive Toxicity

A three-generation reproductive toxicity study was conducted in Sprague-Dawley rats with boric acid. Male and female rats were fed a diet containing 0, 117, 350 or 1,170 ppm boron (approximately 0, 5.9, 17.5 or 58.5 mg B/kg-day, respectively). In the lower two dose groups, there were no treatment-related effects on reproduction. Litter size, progeny weights, fertility, live birth indices, lactation, appearance were similar to the controls. No gross abnormalities were noted in these two dose groups. The 1,170 ppm dose group were found to be sterile, and there were no litters from mating the treated females with control males. Lack of viable sperm was found in the atrophied testes of all 1,170 ppm males. Decreased ovulation was also seen in the majority of the ovaries of the 1,170 ppm females. The NOAEL for this study is 350 ppm boron or approximately 17.5 mg B/kg-day (Weir and Fisher, 1972). [Kl. score = 2]

A three-generation reproductive toxicity study was conducted in Sprague-Dawley rats with borax. Male and female rats were fed a diet containing 0, 117, 350 or 1,170 ppm boron (approximately 0, 5.9, 17.5 or 58.5 mg B/kg-day, respectively). In the lower two dose groups, there were no treatment-related effects on reproduction. Litter size, progeny weights, fertility, live birth indices, lactation, appearance were similar to the controls. No gross abnormalities were noted in these two dose groups. The 1,170 ppm dose group were found to be sterile, and there were no litters from mating the treated females with control males. Lack of viable sperm was found in the atrophied testes of all 1,170 ppm males. Decreased ovulation was also seen in the majority of the ovaries of the 1,170 ppm females. The NOAEL for this study is 350 ppm boron or approximately 17.5 mg B/kg-day (Weir and Fisher, 1972). [Kl. score = 2]

In a continuous breeding protocol, male and female CD-1 mice were given in their diet 0, 1,000, 4,500 or 9,000 ppm boric acid in their feed. The authors estimated that the average daily intakes were: 0, 26.6, 111, and 220 mg B/kg-day to males; and 0, 31.8, 152, 257 mg B/kg-day to females.

Boric acid consumption did not differ among the groups. There were no litters in the 9,000 ppm breeding pairs. At 4,500 ppm, there was a successful first litter, after which there was a progressive decrease in fertility; only one pair produced a fourth and fifth litter. All fertility indices were affected in the 4,500 ppm group. A complete crossover mating trial was conducted using control mice and the 4,500 ppm mice. The results showed that the probable cause of the reduced fertility was a decrement in male fertility. A dose-related decrease in body, testicular and epididymal weights was observed in the 4,500 and 9,000 ppm F_0 males. Sperm count was significantly decreased in these two dose groups, and percent motile sperm was decreased in all dose groups. Testicular histopathology showed seminiferous tubular atrophy in the 9,000 ppm males and partial atrophy of the seminiferous tubules in the 4,500 ppm males. There were no histopathologic changes in the 4,500 ppm females. No statistically significant decreases in mating index, fertility index, or live pups/litter in the 4,500 ppm females, but the number of days to litter in this dose group was increased. Estrous cyclicity was unaffected. Reproductive organ weights were unaffected, but relative maternal liver and kidney/adrenal weights were reduced. An F_1 fertility trial was performed using offspring from the 1,000 ppm groups. There was no decreases in mating, fertility or reproductive performance. The F_2 adjusted live pup weight was slightly, but significantly, reduced from controls. A clear NOAEL for reproductive toxicity in males was not seen in this study. The 1,000 ppm males had decreased sperm motility in the F_0 generation and decreased sperm concentration in the F_1 generation. Decreased F_2 pup relative body weight was statistically significant from controls. The NOAEL in this study for females is 1,000 ppm boric acid or 32 mg B/kg-day). The LOAEL in this study for males is 1,000 ppm or 27 mg B/kg-day; a NOAEL was not established (Fail *et al.* 1991). [Kl. score = 2]

J. Developmental Toxicity

No studies are available on borax.

Pregnant female SD rats were given 0, 0.1, 0.2 or 0.4% boric acid in their feed on gestational days (GD) 0 to 20 or 0.8% boric acid on GD 6 to 15. The average amounts of boric acid ingested were estimated to be 0, 78, 163, 330 or 539 mg/kg-day (0, 13.6, 28.5 or 57.7 mg B/kg-day), respectively. Effects on the pregnant rats were altered food and/or water intake at $\geq$0.2% boric acid, increased liver and kidney weights relative to body weights at $\geq$0.2%, reduced weight gain at $\geq$0.4%, and increased corrected weight gain at 0.4% boric acid. There was a reduction in fetal body weights in all treated groups (94, 87, 63, and 47% of control weight, respectively). Increased malformations occurred at $\geq$0.2%, and prenatal mortality was increased at 0.8%. There was a dose-response for altered skeletal morphology in rats ($\geq$0.1%), and specific findings were significantly elevated above controls at $\geq$0.2%. Specifically, there was an increased incidence of short rib XIII (a malformation) and a decreased incidence or rudimentary or full rib(s) at lumbar I (an anatomical variation) (Heindel *et al.* 1992). [Kl. score = 2]

Pregnant female SD rats were given in their feed 0, 0.025, 0.005, 0.075, 0.1 or 0.2% boric acid on GD 0 to 20. Approximately half of the dams were terminated on GD 20, and the remaining dams delivered their litters. Pup growth and viability were monitored until postnatal day (PND) 21. The average amounts of boron ingested on GD 20 were: 0, 3.3, 6.3, 9.6, 13.3, and 25 mg B/kg-day], respectively. The average amounts of boron ingested on PND 21 were : 0, 3.2, 6.5, 9.7, 12.9, and 25.3 mg B/kg-day, respectively. There were no maternal deaths and no treatment-related clinical signs. Maternal body weights were similar across all groups during gestation. However, decreased maternal body weights (GD 19 and 20 at sacrifice) and decreased maternal body weight gain (GD 15-18 and GD 0-20) were statistically significant in trend tests. There was a 10% reduction in gravid uterine weight (statistically significant) in the 0.2% group. Corrected maternal weight (maternal

gestational weight minus reduced gravid uterine weight) was unaffected by treatment. Feed intake in the 1,000 ppm dams was minimally affected and only during the first three days of dosing. Water consumption was higher in the treated groups after GD 15. The number of corpora lutea and uterine implantation sites, and the percentage of preimplantation loss were similar across all groups. Increased relative kidney weights were increased in the 0.2% group. There were no differences in the viability of the offspring between treated and controls. On GD 20, fetal body weight was 94% and 88% of controls in the 0.1% and 0.2% groups, respectively; recovery was complete at birth (~GD 22). The incidence of short rib XIII was increased on GD 20 in the ≥0.1% groups, but only in the 0.2% group at PND 21. The incidence of wavy rib was increased on GD 20 in the ≥0.1% group; the reversibility of this effect was confirmed on PND 21. There was a slight decrease in extra lumbar ribs in the 0.2% group on GD 20, and extra lumbar ribs were seen in the 0.2% group on PND 21. The developmental NOAEL was considered to be 0.075% boric acid or 9.6 mg B/kg-day on GD 20; and 0.1% boric acid or 12.9 mg B/kg-day on PND 21 (Price *et al.* 1996a). [Kl. score = 1]

Pregnant Swiss mice were given in their diet 0, 0.1, 0.2 or 0.4% boric acid on gestational days (GD) 0 to 17. The average amounts of boric acid ingested were estimated to be 248, 452 or 1,003 mg/kg-day (0, 43.4, 79.0 or 175.3 mg/B/kg-day), respectively. Maternal toxicity consisted of mild kidney lesions (≥0.1%), increased water intake and relative kidney weights (0.4%), and decreased water intake during treatment. Fetal body weights were reduced in the ≥0.2% groups, and there were increased incidences of resorptions and malformed fetuses per litter in the 0.4% group. The LOAEL for maternal toxicity is 248 mg/kg-day boric acid or 43.4 mg B/kg-day; a NOAEL was not established. The NOAEL for developmental toxicity is 248 mg/kg-day boric acid or 43.4 mg B/kg-day (Heindel *et al.* 1992). [Kl. score = 2]

Pregnant female New Zealand rabbits were dosed by oral gavage with 0, 62.5, 125 or 250 mg/kg boric acid (0, 10.9, 21.9 or 43.7 mg B/kg) during GD 6-19. Feed intake was in the 250 mg/kg maternal animals during the exposure period, but it was increased in the ≥125 mg/kg dose groups. In the 250 mg/kg group, maternal body weights during GD 9-30, weight gain during GD 6-19, gravid uterine weight, and number of corpora lutea per dam were significantly reduced. In the ≥125 mg/kg groups, maternal corrected gestational weight gain was increased compared to controls. Maternal liver weights were unaffected by treatment. In the 250 mg/kg group, relative, but not absolute, kidney weights were increased, although no effects in the kidney were noted in the histopathological examination. Prenatal mortality was increased in the 250 mg/kg group (90% resorptions/litter versus 6% for controls); the proportion of pregnant females with no live fetuses was increased (73% versus 0%), and live litter size was reduced (2.3 fetuses versus 8.8). Thus, there were only 14 live fetuses (6 live litters) available for evaluation in the 250 mg/kg group. The percentage malformed fetuses/litter was increased in the 250 mg/kg group, primarily due to cardiovascular defects (72% versus 3% of controls). There was no definitive maternal or developmental toxicity in the 62.5 or 125 mg/kg dose groups. The NOAEL for maternal and developmental toxicity is 125 mg/kg-day boric acid or 21.9 mg B/kg-day (Price *et al.* 1996b). [Kl. score = 1]

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for boric acid follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2021).

Non-Cancer

An oral reference dose was not derived for boric acid or borax.

The Australian drinking water guideline value for boron (4 mg/L) may be applicable (ADWG, 2021). The health-based ADWG value was based on a tolerable daily intake (TDI) of 0.16 mg/kg bw. This TDI is based on the NOAEL of 9.6 mg/kg bw/day for foetal bodyweight effects in a rat developmental study (Price et al. 1996a) with an uncertainty factor of 60 (10 for interspecies and 6 for human intraspecies).

Cancer

There was no evidence of carcinogenicity in rat and mouse chronic studies conducted on borax and/or boric acid. Thus, a cancer reference value was not derived.

L. Human Health Hazard Assessment of Physico-Chemical Properties

Borax and boric acid do not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing potential

7. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Borax and boric acid have low acute and chronic toxicity to aquatic organisms.

B. Aquatic Toxicity

In ecotoxicological tests for boron, the exposure concentrations are expressed as boron equivalents i.e., mg B/L. This is because boric acid and borate salts will have the same boron speciation when dissolved in environmental matrices. Therefore, in the following sections toxicological values are given as mg B/L regardless of the form of boron that was tested.

Acute Studies

Borax will transform into boric acid in the aquatic environment. Table 4 lists the results of acute aquatic toxicity studies conducted on boric acid.

Table 4: Acute Aquatic Toxicity Studies on Boric Acid

Test Species	Endpoint	Results (mg B/L)	Klimisch score	Reference
Fathead minnow	96-hr LC_{50}	79.7	2	ECHA
Legumia recta (Black sandshell mussel)	96-hr LC_{50}	147	2	ECHA
Hyalella azteca	96-hr LC_{50}	64	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	52.4 mg B/L	1	ECHA

Chronic Studies

Long-term effects (LC_{10}) on freshwater fish ranged from 3.5 to 47 mg B/L. Adequate long-term LC_{10} of 21.6 mg B/L was found for the fresh water fish *P. promelas* in a study according to EPA OPPTS 850.1400 (ECHA) [Kl. Score = 2].

Long-term effects (LC10/NOEC) on reproduction on freshwater vertebrates ranged from 6.6 to 32 mg B/L based on several well-accepted guideline studies (ECHA) [Kl. Scores =1 or 2].

Boric acid has been evaluated for its toxicity towards the fresh water alga *Pseudokirchneriella subcapitata* (formerly *Selenastrum capricornutum*) in an Alga growth inhibition test according to OECD 201 under GLP requirements. The exposure duration was 72 hours under static conditions. The NOEC growth rate determined from the study was 17.5 mg B/L (ECHA) [Kl. Score = 1].

The ANZG water quality guideline (2021) derived a very high reliability default guideline value (DGVs) for (dissolved) boron in freshwater from 22 chronic (long-term) toxicity data, comprising eight fish, two amphibians, three crustaceans, one bivalve, three macrophytes, one green microalga, three diatoms and one blue–green alga. The summary of representative data used by ANZG to develop a water quality guideline for boron is presented in Table 5 below. These values are noted to be consistent with those reported in ECHA. Additional chronic aquatic toxicity data is found in the ANZG Technical Brief (ANZG, 2021).

Table 5: Chronic Aquatic Toxicity Studies on Boron[1]

Test Species	Endpoint	Results (mg B/L)
Danio rerio	34-day NOEC (Biomass)	1.8
Pimephales promelas	32-day NOEC (Mortality)	11
Daphnia magna	14-day NOEC (Reproduction)	2.4
Pseudokirchneriella subcapitata	4-day NOEC (Growth)	2.8

1 - The DGVs are based on toxicity data for boron as either boric acid, H_3BO_3 (CAS 10043-35-3), or borax, $Na_2B_4O_710H_2O$ (CAS 1303-96-4), in freshwater.

In the chronic toxicity data set, fish sensitivity to boron ranged from the least sensitive species in the dataset (*Melanotaenia splendida*, LC10 102 mg/L) to the third most sensitive species in the dataset (*Danio rerio*, NOEC 1.8 mg/L). Of the crustaceans, *D. magna* was best represented in the literature, with 18 published NOEC values (ranging from 2.4 mg/L to 29 mg/L) for six different endpoints from

six different publications. The final NOEC of 2.4 mg/L used in the DGV derivation was lower than that for *C. dubia* (NOEC 5.6 mg/L) and for the amphipod *H. azteca* (NOEC 6.6 mg/L).For *P. subcapitata*, there were three separate studies available with toxicity data for boron. The toxicity values from these studies ranged from a NOEC of 2.8 mg/L to a NEC of 27 mg/L, varying with endpoint, duration and test medium used. Boron was least toxic to *P. subcapitata* when tested in algal growth medium with added $NaHCO_3$, suggesting that carbonate addition may have influenced boron toxicity. Therefore, although NECs are preferred to NOECs or EC10s (Warne et al. 2018), in this instance, a reliable NOEC of 2.8 mg/L was the most sensitive toxicity value for *P. subcapitata* (ANZG, 2021).

C. Sediment Toxicity

Limited sediment toxicity data are available for boric acid and boron containing compounds in general (NICNAS, 2019).

Chronic toxicity values for the effects of boric acid on sediment-dwelling invertebrates have been obtained for a freshwater midge (*Chironomus riparius*, harlequin fly), a freshwater bivalve (*Lampsilis siliquoidea*, fatmucket clam), and the aquatic worm (*Lumbriculus variegatus,* California blackworm). The respective toxicity values for these species are as follows: 28 d NOEC = 37.8 mg B/kg; 21 d LC25 (survival) = 363.1 mg B/kg; and 28 d NOEC = 100.8 mg B/kg (NICNAS, 2019).

Due to the high water solubility of boron and its low partitioning to sediment, sediment toxicity testing for boron is particularly challenging as it is difficult to ensure that exposure is through the solid phase (i.e., sediment) and not from the aqueous boric acid in the overlying water (NICNAS, 2019).

D. Terrestrial Toxicity

Ecotoxicological tests with plants and soil invertebrates have recorded modest chronic toxicity values (NOECs/ECs) in the range of 15.3 to 84.0 and 5.2 to 315 mg total B/kg, respectively (ECHA, 2008). However, to predict the potential toxicity of boron to plants and soil organisms, measuring the total boron concentration may be unsuitable. Instead, potential toxicity is better predicted using boron concentrations in the soil solution (extractable boron) (Mertens, et al., 2011). In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron (NICNAS, 2019).

E. Calculation of PNEC

<u>PNEC water</u>

The ANZG water quality guideline (2021) derived a very high reliability DGV for (dissolved) boron in freshwater. The DGVs for 99, 95, 90 and 80% species protection are 340 µg/L, 940 µg/L, 1,500 µg/L and 2,500 µg/L, respectively. The 95% species protection level for boron in freshwater (940 µg/L) is recommended for adoption in the assessment of slightly-to-moderately disturbed ecosystems. (ANZG, 2021).

<u>PNEC sediment</u>

Limited sediment toxicity data are available for boric acid and boron containing compounds in general (NICNAS, 2019). Due to the high water solubility of boron and its low partitioning to sediment, sediment toxicity testing for boron is particularly challenging as it is difficult to ensure that

exposure is through the solid phase (i.e., sediment) and not from the aqueous boric acid in the overlying water (NICNAS, 2019). K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as boric acid and borax. Therefore, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. As a result, the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

In the ECHA REACH database (ECHA), a $PNEC_{soil}$ was derived for boron using the species sensitivity distribution method and an assessment factor of 2. The $PNEC_{soil}$ was determined to be 5.7 mg/kg soil dry weight.

8. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Borax is an inorganic compound that dissociates completely to boric acid and the borate anion in aqueous media. Biodegradation is not applicable to these inorganic compounds; both boric acid and borate are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable.

A BCF of <0.1-10.5 L/kg has been reported for borates in fish and oysters. This data suggests that boric acid does not bioaccumulate in the aquatic environment. Thus, boric acid and borax do not meet the criteria for bioaccumulation.

The chronic toxicity data on boric acid has a NOEC > 0.1 mg/L. Acute $E(L)C_{50}$ values are > 1 mg/L. Thus, borax and boric acid do not meet the criteria for toxicity.

The overall conclusion is that borax and boric acid are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for borax or boric acid.

9. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Boric Acid	10043-35-3	Not a PBT	Yes	No	NA	No	No	No	1	1	2
Sodium Tetraborate Decahydrate (Borax)	1303-96-4	Not a PBT	Yes	No	NA	No	No	No	1	1	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry

kg	kilograms
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NEC	no effect concentration
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

Qualitative Tier 2 Assessment

C10-C16 Alkylbenzenesulfonic Acid

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

C10-C16 alkylbenzenesulfonic acid is a component in the KCl/Polymer Stuck Pipe Mud system. The secondary mud system is used to free stuck pipes and, as a secondary mud, will only be used as required. As a result, these secondary muds are considered insignificant relative to the primary muds due to the considerably reduced volume used (<0.1%) as compared to the other muds. The purpose and maximum quantity (i.e., in all muds) for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
C10-C16 Alkylbenzenesulfonic acid	68584-22-5	Emulsifier	NA

[1] Based on maximum of combined muds assessed
CAS No = Chemical Abstracts Service Number
NA = quantity used varies with severity of loss

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on C10-C16 alkylbenzenesulfonic acid, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	2-year rat dietary	None	250	100	2.5	9

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	-	-	-	0.28[a]

[a] $PNEC_{water}$ for C10-C16 alkylbenzenesulfonic acid is the ANZG Water Quality Guideline – Freshwater Trigger Value for Linear Alkylbenzene Sulfonate.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	[a]	-	-	27

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	[a]	-	-	24

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

C10-C16 alkylbenzenesulfonic acid has an average alkyl chain length of 11.3 to 11.8 (HPVIS). This range includes benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives sulfonic acid (CAS No. 85536-14-7). The molecular structure of C10-C16 alkylbenzenesulfonic acid is presented in **Figure 1**.

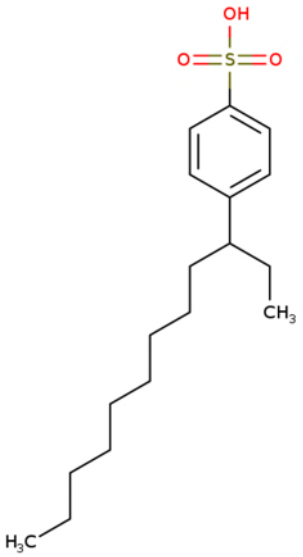

Figure 1 Molecular Structure of C10-C16 Alkylbenzenesulfonic Acid[2]

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. It has a low-to-moderate potential for bioaccumulation based on structurally similar compounds.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for C10-C16 alkylbenzenesulfonic acid is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that C10-C16 alkylbenzenesulfonic acid is not a PBT substance.

Human Health Hazards

C10-C16 alkylbenzenesulfonic acid exhibits moderate acute toxicity by the oral route and low acute toxicity by the dermal route. The following information was derived from products of similar structure or composition. It is highly irritating to the skin and eyes, but not a skin sensitiser. No systemic, reproductive or developmental toxicity was seen. It is not genotoxic.

There are no repeated-dose toxicity studies on C10-C16 alkylbenzenesulfonic acid. However, a reliable two-year dietary study was conducted in rats on C10-C14 Linear Alkylbenzene Sulfonate (CAS No. 69669-44-9). In this study, there were no treatment-related effects with a no observed adverse effect level (NOAEL) of 250 milligrams per kilogram-day (mg/kg-day) (Buehler et al., 1971). This NOAEL was used for determining the oral RfD and the drinking water guideline value (9 mg/L) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

C10-C16 alkylbenzenesulfonic acid may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/68584-22-5

There is low potential for human receptors to be exposed to C10-C16 alkylbenzenesulfonic acid in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, C10-C16 alkylbenzenesulfonic acid is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), database indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, C10-C16 alkylbenzenesulfonic acid is a moderate toxicity concern to aquatic organisms. Acute toxicity towards fish and aquatic invertebrates is of the same order of magnitude. However, algae (*Scenedesmus subspicatus)* was somewhat less sensitive (ECHA).

C10-C16 alkylbenzenesulfonic acid is biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for C10-C16 alkylbenzenesulfonic acid are provided in **Tables 3 – 5**. The C10-C16 alkylbenzenesulfonic acid is a Linear Alkylbenzene Sulfonate (LAS). ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 0.28 mg/L for LAS. This value, which was identified as the PNEC for water (see **Table 3**), was derived using data normalised to an alkyl chain length of C11.6 using the statistical distribution method with 95% protection.

There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method (see **Tables 4 and 5**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of C10-C16 alkylbenzenesulfonic acid in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of C10-C16 alkylbenzenesulfonic acid in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as C10-C16 alkylbenzenesulfonic acid, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days..

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

References

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ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

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HPVIS. United States Environmental Protection Agency High Production Volume Information System (HPVIS): https://iaspub.epa.gov/oppthpv/public_search.html_page.

Attachment 1 Risk Assessment Dossier

C10 –C16 ALKYLBENZENESULFONIC ACID

This dossier on C10-C16 alkylbenzenesulfonic acid presents the most critical studies pertinent to the risk assessment of C10-C16 alkylbenzenesulfonic acid in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the United States Environmental Protection Agency High Production Volume Information System (HPVIS) Chemical Challenge Program. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – C10-C16 alkylbenzenesulfonic acid was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. C10-C16 alkylbenzenesulfonic acid was assessed as a tier 2 chemical for acute toxicity. Therefore, C10-C16 alkylbenzenesulfonic acid is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. It has a low-to-moderate potential for bioaccumulation based on structurally similar compounds. C10-C16 alkylbenzenesulfonic acid exhibits moderate acute toxicity by the oral route and low acute toxicity by the dermal route. The following information was derived from products of similar structure or composition. It is highly irritating to the skin and eyes, but not a skin sensitiser. Repeated oral toxicity studies have shown no target organ effects. It is not genotoxic, and animal dietary studies showed no indication of adverse reproductive or developmental effects. C10-C16 alkylbenzenesulfonic acid is of moderate toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC):
petroleum, di-C10-16 linear saturated alkaryl derivatised Benzenesulfonic acids
CAS RN: 68584-22-5
Molecular formula: variable
Molecular weight: variable

Synonyms: p-dodecylbenzenesulfonic acid; Benzenesulfonic acid, 4-dodecyl-4-Dodecylbenzene-1-sulfonic acid; 4-Dodecylbenzenesulphonic acid (mixed isomers)

C10-C16 alkylbenzenesulfonic acid (CAS No. 68584-22-5) has an average alkyl chain length of 11.3 to 11.8 (HPVIS). This range includes benzenesulfonic acid, 4-C10-13-sec-alkyl derivs. sulfonic acid (CAS No. 85536-14-7).

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of C10-C16 Alkylbenzenesulfonic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Brown, viscous liquid	-	ECHA
Melting Point	334 °C @ 101.3 kPa	2	ECHA
Boiling Point	1043 °C @ 101.3 kPa	2	ECHA
Density	-	-	-
Vapor Pressure	2.89 x 10^{-8} Pa (estimated) (temperature not provided)	2	HPVIS
Partition Coefficient (log K_{ow})	22 @ 25°C	2	ECHA
Water Solubility	0 g/L @ 25°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for C10-C16 alkylbenzenesulfonic acid.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. It is insoluble in water and has a high potential for adsorption to soil or sediments. It has a low-to-moderate potential for bioaccumulation based on structurally similar compounds.

B. Partitioning

Based on its vapour pressure, volatilisation is not expected to be an important fate and transport pathway.

C. Biodegradation

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. In an OECD DOC Die-away test, benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) was degraded 94% after 28 days (HPVIS) [Kl. score = 1]. In a modified coupled units test, benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) was degraded 92% after 37 days (HPVIS) [Kl. score = 1].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental studies are available for C10-C16 alkylbenzenesulfonic acid. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} values for various surrogates of C10-C16 alkylbenzenesulfonic acids are presented in Table 3 which indicate that these compounds are expected to have the potential for low to slight mobility or even immobility (Koc >5,000) in soil. I If released to water, based on these K_{oc} values and the substance's insolubility, it would likely also adsorb to suspended solids or sediment.

Table 3 K_{oc} Values for Surrogates of C10-C16 Alkylbenzenesulfonic Acid

Substance	K_{oc} (MCI estimate)	K_{oc} (log K_{ow} estimate)
4-(1-ethyloctyl)-benzenesulfonic acid	3,505 L/kg	973.4 L/kg
4-(1-ethylnonyl)-benzenesulfonic acid [CAS No. 18777-52-1]	6,388 L/kg	1,817 L/kg
4-(1-ethyltetradecyl)-benzenesulfonic acid	128,400 L/kg	41,690 L/kg

E. Bioaccumulation

No experimental studies are available for C10-C16 alkylbenzenesulfonic acid. Bioconcentration of C10-C16 alkylbenzenesulfonic acid in aquatic organisms is not expected to occur based on a measured log K_{ow} of 2.0 (HPVIS).

A bioconcentration fish (OECD 305 E) study was conducted on C10-C13 Linear Alkylbenzene Sulfonate (LAS). The BCF values ranged between 2 and 1,000 L/kg, with BCFs increasing with increasing alkyl chain length. To address differences in composition of mixtures, bioconcentration potential was evaluated for a mixture typical of LAS in European detergent formulations (C10 12%, C11 29%, C12 34%, C13 24%); average alkyl chain length – C11.6 and a mixture typical of LAS in filtered Mississippi river water (C10 45%, C11 23%, C12 23%, C13 2%; average chain length = C10.8). The respective BCFs were 87 and 22 L/kg at concentrations of 2.7 and 4.1 µM (HPVIS). [Kl. score = 2]

A BCF of 130 was reported for *Leuciscus idus melanotus* in a 3-day test conducted on dodecylbenzenesulfate, sodium salt (HPVIS). [Kl. score = 1]

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

C10-C16 alkylbenzenesulfonic acid exhibits moderate acute toxicity by the oral route and low acute toxicity by the dermal route. The following information was derived from products of similar structure or composition. It is highly irritating to the skin and eyes, but not a skin sensitiser. Repeated oral toxicity studies have shown no target organ effects. It is not genotoxic, and animal dietary studies showed no indication of adverse reproductive or developmental effects.

B. Acute Toxicity

The oral LD_{50} in rats for the C10-C16 alkylbenzenesulfonic acid is 775 mg/kg (HPVIS) [Kl. score = 1]. The oral LD_{50} in rats for the benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) is 1,470 mg/kg (HPVIS). [Kl. score = 1]

The dermal LD_{50} in rabbits for C10-C16 alkylbenzenesulfonic acid is 2,000 mg/kg (HPVIS). [Kl. score = 1]

C. Irritation

No studies are available on C10-C16 alkylbenzenesulfonic acid.

Application of 0.5 mL benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) to the skin of rabbits for four hours was highly irritating. The irritation index was 5.25 (HPVIS). [Kl. score = 1]

Instillation of 0.1 ml benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) into the eyes of rabbits was moderately irritating. The primary irritation index was 46.9 (HPVIS). [Kl. score = 1]

D. Sensitisation

No studies are available on C10-C16 alkylbenzenesulfonic acid.

A C10-C13 benzenesulfonic acid was not considered a skin sensitiser in a guinea pig maximisation test (HPVIS). [Kl. score = 1]

E. Repeated Dose Toxicity

No studies are available for C10-C16 alkylbenzenesulfonic acid.

Oral

Male and female Wistar rats were given feed containing 0, 0.07, 0.2, 0.6 or 1.8% C10-C14 alkylbenzenesulfonic acid for six months. The 1.8% group had diarrhea, markedly depressed growth, increased cecal weight and marked degeneration of the renal tubules. The 0.6% group had slightly depressed growth, increased cecal weight, increased serum alkaline phosphatase activity, decreased serum protein and degeneration of the renal tubules. The 0.2% group had increased cecal weight and slight degeneration of the renal tubules. The 0.07% group showed no treatment-related effects. The NOAEL was reported to be 0.07%, which was estimated to be 40 mg/kg-day (Yoneyama *et al.*, 1972; IPCS 1996). [Kl. score = 4]

Male and female Wistar rats were given feed containing 0, 0.04, 0.16 or 0.6% C10-C14 alkylbenzenesulfonic acid for up to 24 months. The 0.6% group had slightly increased live and cecal weights, and increased activity of serum glutamate-pyruvate transaminase and alkaline phosphatase. There were no treatment-related effects on food consumption, body weight gain, clinical signs, mortality or mean survival. The NOAEL was considered to be 0.6%, which was estimated to be 300 mg/kg-day (Yoneyama et al., 1977; IPCS, 1996). [Kl. score = 4]

Male and female CR rats were given feed containing 0, 0.02, 0.1 or 0.5% C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9) for two years. The mean daily intakes were estimated to be 0, 10, 50 and 250 mg/kg-day. Body weight gain and feed consumption were similar across all groups. There were no treatment-related effects on hematology parameters in the gross pathology or histopathology examination. The NOAEL is 250 mg/kg-day (Buehler et al., 1971; HPVIS). [Kl score = 2]

Inhalation

No studies are available.

Dermal

No studies are available.

F. Genotoxicity

In Vitro Studies

C10-C16 alkylbenzenesulfonic acid was not mutagenic to *S. typhimurium* strains TA98 and TA100 in the absence or presence of metabolic activation (HPVIS). [Kl. score = 1]

In Vivo Studies

Male and female NMRI mice were dosed by oral gavage with a single dose of 0 or 1,122 mg/kg benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7). There were no significant increases in the number of micronucleated polychromatic erythrocytes in bone marrow cells (HPVIS). [Kl. score = 1]

Male and female ICR: JCL mice were dosed by oral gavage with 0, 200, 400 or 800 mg/kg C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9) either as a single dose or given a single daily dose for 5 consecutive days. There were no significant increases in the number of chromosomal aberrations in bone marrow cells (HPVIS). [Kl. score = 1]

G. Carcinogenicity

Oral Studies

No studies are available on C10-C16 alkylbenzenesulfonic acid.

Male and female CR rats were given feed containing 0, 0.02, 0.1 or 0.5% C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9) for two years. The mean daily intakes were estimated to be 0, 10, 50 and 250 mg/kg-day. Body weight gain and feed consumption were similar across all groups. The incidence of tumours in the treated animals were similar to the controls (Buehler et al., 1971; HPVIS). [Kl score = 2]

H. Reproductive Toxicity

No studies are available on C10-C16 alkylbenzenesulfonic acid.

A reproductive toxicity study was conducted on C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9). The dietary doses were 0, 0,02, 0.1 or 0.5%, which were estimated to be 0, 14, 70 and 350 mg/kg-day, respectively. The P0 generation were fed for 84 days; when 107-112 days old, females from each dose group were mated with males from the same group and maintained together for 17 days. The first litters of each generation (F1a- and F2a-generation) were sacrificed at 21 days of age. Ten days after the final litter was sacrificed, all females were re-mated with different males from the same group to obtain the F1b generation. From the F1b generation, males and females of each group were selected at weaning to continue their respective diets and to be used for further reproduction studies. Reproduction studies on the F1b and F2b generations were started when the rats were 80-85 days old, and were continued until the F3b generation was weaned. There were no treatment-related effects on fertility, gestation, parturition, neonatal viability, lactation, and post-weaning growth. The NOAEL for reproductive toxicity is 350 mg/kg-day, the highest dose tested (Buehler et al., 1971; HPVIS). [Kl. score = 2]

I. Developmental Toxicity

No studies are available on C10-C16 alkylbenzenesulfonic acid.

Pregnant female SD-JCL rats were given in their feed 0, 0.1 or 1.0% Linear Alkylbenzene Sulfonate (average alkyl chain length = C11.7 to C12.3) on GD 0 to 20. Body weight gain in the dams were similar between treated and control groups, and there was no treatment-related effects on the occurrence and maintenance of pregnancy. The litter parameter values were similar across all groups and there was no evidence of teratogenicity. In the 1% group, the numbers of offspring were low and the weaning rate was 78.3% compared to the rate in the controls (100%). There were no adverse effects in the offspring body weight gain, organ weights or function. The NOAEL for maternal and developmental toxicity is considered to be 1% in the diet (calculated to be 780 mg/kg-day) (Tiba et al., 1976; HPVIS). [Kl. score = 4]

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for C10-C16 alkylbenzenesulfonic acid follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

There are no repeated-dose toxicity studies on C10-C16 alkylbenzenesulfonic acid (CAS No. 68584-22-5). However, a reliable (Kl. score = 2) two-year dietary study was conducted in rats on C10-C14 Linear Alkylbenzene Sulfonate (CAS No. 69669-44-9). In this study, there were no treatment-related effects with a NOAEL of 250 mg/kg-day (Buehler et al., 1971 as cited in OECD 2005). This study is supported by another two-year rat dietary study conducted on C10-C14 alkylbenzenesulfonic acid, which was published in a Japanese journal and was summarised in IPCS (1996); the NOAEL from this study was considered to be 300 mg/kg-day.

The NOAEL of 250 mg/kg-day from Buehler *et al.*, (1971) (as cited in OECD 2005) will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 250/(10 x 10 x 1 x 1 x 1) = 250/100 = 2.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (2.5 x 70 x 0.1)/2 = 9 mg/L

Cancer

No carcinogenicity studies are available on C10-C16 alkylbenzenesulfonic acid. However, a chronic dietary study was conducted in rats on C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9), which has a similar composition to C10-C16 alkylbenzenesulfonic acid. There were no carcinogenic effects in this dietary study. Therefore, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

C10-C16 alkylbenzenesulfonic acid does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

C10-C16 alkylbenzenesulfonic acid is of moderate toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on C10-C16 alkylbenzenesulfonic acid.

Table 4 Acute Aquatic Toxicity Studies on C10-C16 Alkylbenzenesulfonic Acid

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Cyprinus carpio	96-hour LC_{50}	5.6*	1	HPVIS
Daphnia magna	48-hour EC_{50}	5.2*	1	HPVIS
Daphnia magna	48-hour EC_{50}	9.3 – 11.6**	1	HPVIS
Daphnia magna	48-hour EC_{50}	2.9	1	HPVIS

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Scenedesmus subspicatus	72-hour EC_{50}	36* (growth rate)	1	HPVIS
Scenedesmus subspicatus	EC_{50}	170***	1	HPVIS

*Benzenesulfonic acid, C10-C13-alkyl derivatives

**Three Linear Sulfonic Acids (LAB) of varying chain lengths were neutralised with caustic soda to obtain the sodium salt derivative. Acid A had 48.4% of its weight in the C11 range and the majority of its chain length ranged from C10-C13. Acid B had a 49.4% of its weight in the C11 range and 31.7% of its weight in the C12 range. The majority of its chain length ranged from C10 to C12. Acid C had the majority of its chain length in the C10 to C13 range, almost evenly distributed between C11 and C12. The LC_{50} values were 11.6, 10.8 and 9.3 for Acids A, B and C, respectively.

***C10-C13 linear alkyl benzenesulfonic acid

Chronic Studies

The 28-day chronic toxicity of a commercial C10-C13 Linear Alkylbenzene Sulfonate (average carbon lengths of C11.6 and C11.8) was tested in several species of fish. The NOEC values were normalised using QSARs to the average structure of C11.6 Linear Alkylbenzene Sulfonate. The geometric mean NOECs (and the number of studies) for the various fish species are as follows: 2.3 mg/L for *Brachydanio rerio* (n=1); 0.87 mg/L for *Pimephales promelas* (n=14); 0.34 mg/L for *Oncorhynchus mykiss* (n=7); and 0.25 mg/L for *Tilapia mossambica* (n=1) (HPVIS). [Kl. score = 4].In a chronic *Daphnia* study, the NOEC of the geometric mean of 12 records compiled from the literature review and the LAS normalised to C11.6 was 1.4 mg/L (HPVIS). [Kl. score = 4]. The low Klimisch ratings for these studies make them unsuitable for risk categorization.

C. Terrestrial Toxicity

No adequate information is available.

D. Calculation of PNEC

The C10-C16 alkylbenzenesulfonate is a Linear Alkylbenzene Sulfonate (LAS).

ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 280 µg/L for LAS. This value was derived using data normalised to an alkyl chain length of C11.6 using the statistical distribution method with 95% protection.

The data set that was used included the following:

Freshwater fish: 5 species, 250 to 3,200 µg/L.

Freshwater crustaceans: 2 species, 1,400−3,200 µg/L.

Freshwater insects: 2 species, 2,800−3,400 µg/L.

Freshwater mesocosms: NOEC of 300 µg/L by Guhl and Gode (1989), an OECD guideline study.

Freshwater algae: 6 species, 80−15, 000 µg/L

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 27 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (123.4/1280) \times 1000 \times 0.28$
$= 27$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 255.5/1000 \times 2400]$
$= 123.4\ m^3/m^3$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 6{,}388 \times 0.04$
$= 255.5$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for C10-C16 alkylbenzenesulfonate calculated from EPISUITE™ using MCI and the surrogate 4-(1-ethylnonyl)-benzenesulfonic acid is 6,388 L/kg. As discussed in Section 5, the K_{oc} value for this substance ranges from 3,505 L/kg to 128,404 L/kg. The PNEC value is directly related to this value. Thus, a lower K_{oc} would result in a lower PNEC and vice versa.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 24 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (127.8/1500) \times 1000 \times 0.28$
$= 24$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$Kp_{soil} = K_{oc} \times f_{oc}$
= 6,388 x 0.02
= 127.8 m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for C10-C16 alkylbenzenesulfonate calculated from EPISUITE™ using MCI and the surrogate 4-(1-ethylnonyl)-benzenesulfonic acid is 6,388 L/kg. As noted, above the K_{oc} value for this substance is variable.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable; thus it does not meet the screening criteria for persistence.

The experimental BCFs for several linear alkylbenzene sulfonates that are structurally related to C10-C16 alkylbenzenesulfonate range from 22 to 130; thus, C10-C16 alkylbenzenesulfonic acid does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on C10-C16 alkylbenzenesulfonic acid show NOECs of >0.1 mg/L. Thus, C10-C16 alkylbenzenesulfonate does not meet the screening criteria for toxicity.

The overall conclusion is that C10-C16 alkylbenzenesulfonic acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for C10-C16 alkylbenzenesulfonic acid.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
C10-C16 alkylbenzenesulfonic acid	68584-22-5	Not a PBT	No	No	No	No	No	No	2	Insufficient data quality for categorisation	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
GD	Gestational day
HHRA	enHealth Human Risk Assessment
HPV	High Production Volume
HPVIS	High Production Volume Information System
IUPAC	International Union of Pure and Applied Chemistry

kg	kilogram
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LAS	Linear Alkyl Sulfonate
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
µg/L	micrograms per litre
µM	micromolar

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
C10-C16 Alkylbenzenesulfonic acid	68584-22-5	1.00E+00	1.50E+01	1.00E-01	2.50E-02	1.00E-03	2.50E-04	2.00E-05	5.00E-06	2.80E-01

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Calcium Carbide

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

During a carbide lag test, calcium carbide reacts with water in the drilling fluid rapidly producing calcium hydroxide and acetylene gas. Acetylene is commonly used as a tracer gas for this purpose. It circulates with the drilling fluid until it reaches the surface, where it is detected and captured at the gas trap. The carbide lag test is used to calculate drill cuttings sample lag.

The purpose and maximum quantity for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity
Calcium carbide	75-20-7	Carbide Lag Test	NA

CAS No = Chemical Abstracts Service Number
NA = quantity used varies with test

The assessment of toxicity of calcium carbide was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. In the environment, decomposition product calcium hydroxide will dissociate into calcium (Ca^{2+}) and hydroxyl (OH^-) ions. The behaviour of hydroxyl ions depends on the pH buffer capacity of the tested medium. Acetylene, as a gas, will not remain in water. The Australian Drinking Water Guidelines (ADWG) doesn't have a limit on health or aesthetics for calcium. However, an ADWG Value is available for hardness (as calcium carbonate) and pH (see **Table 2**), which may be applicable due to presence of Ca^{2+} and OH^- ions. A toxicological reference values (TRV) was not derived for calcium carbide. A detailed discussion of the drinking water guideline value is presented in **Attachment 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Calcium carbide (CAS No. 75-20-7)	Hardness (as calcium carbonate) pH	200 mg/L 6.5 to 8.5

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil were not calculated for the chemical. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Calcium carbide (CAS No. 75-20-7)	*Daphnia magna*	4.62	1000	0.0046

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Calcium carbide is an inorganic substance with a garlic-like odour. The molecular structure for calcium carbide is presented in **Figure 1**.

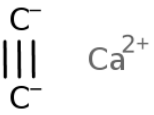

Figure 1 Molecular Structure of Calcium Carbide[2]

In contact with water, calcium carbide instantly decomposes hydrolytically, yielding acetylene gas (CAS No. 74-86-2) and calcium hydroxide (CAS No. 1305-62-0). The hydrolysis half-life for calcium carbide is less than 1 minute.

Decomposition product calcium hydroxide is an inorganic compound. It is partially soluble in water, dissociating into Ca^{2+} and OH^- ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues.

Decomposition product acetylene is a flammable, colourless, gas that is soluble in water. As acetylene is a gas at standard temperature and pressure, biodegradation is not considered relevant. It is not expected to bioaccumulate and has a low potential to adsorb to soil or suspended sediments. Volatilisation is expected to be an important fate process.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for calcium carbide is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

Calcium carbide and its decomposition products have low acute toxicity by oral, dermal, and inhalation routes of exposure. It is a skin and eye irritant but does not have sensitising properties. Several epidemiological studies have identified decomposition product calcium hydroxide/calcium oxide as a respiratory irritant. Any systemic effects of calcium carbide are considered to be negligible at normal occupational exposures. Calcium carbide and its decomposition products are not genotoxic or carcinogenic and do not exhibit developmental or reproductive toxicity.

As noted earlier, in aqueous solution, calcium carbide rapidly decomposes into calcium hydroxide and acetylene. Calcium hydroxide dissociates into calcium and hydroxyl ions. As hydroxyl ions are readily buffered in biological tissue, only calcium ions and gaseous acetylene need to be assessed for systemic adverse effects. Calcium is the most abundant mineral in the human body and part of the normal diet (approx 700 mg/day; ECHA). The second decomposition product, acetylene, has been

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/75-20-7

used for over 100 years as an anaesthetic and as an industrial chemical, and few complications of using this gas have surfaced (ECHA).

A TRV was not derived for calcium carbide. The ADWG value for hardness (as calcium carbonate) is 200 mg/L. The ADWG value for pH is 6.5 to 8.5. Both values are based on aesthetics (see **Table 2**). A detailed discussion of the drinking water guideline values is presented in **Attachment 1**.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents. As previously discussed, calcium carbide instantly decomposes hydrolytically with a hydrolysis half-life of less than 1 minute. As a result, this chemical would not be present in treated water. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

In standard aquatic toxicity tests, calcium carbide is moderately toxic to aquatic organisms. Acute toxicity towards algae and fish is of the same order of magnitude. However, *Daphnia magna* was somewhat more sensitive compared to fish and algae (ECHA).

Studies on the acute toxicity to aquatic invertebrates, algae and fish were conducted with technical calcium carbide. Therefore, effects reported in these studies can be attributed to the entirety of the decomposition products of technical calcium carbide, i.e., calcium hydroxide and acetylene, including any impurities of the technical material (ECHA).

Calcium carbide and its decomposition products are not expected to bioaccumulate. Acetylene is a gas which will not remain in the aqueous phase due to its high vapour pressure and Henry's Law constant. Calcium is a ubiquitous integral part of almost all naturally occurring mineral matrices, in particular of soils and sediments. Also, natural waters carry a significant level of calcium background concentrations. The calcium released from calcium carbide is therefore of no environmental concern (ECHA).

PNECs for calcium carbide are provided in **Table 3**. Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNEC in water. However, there are no toxicity data for sediment-dwelling organisms or soil organisms. Equilibrium partitioning methods cannot be used to calculate PNECs for inorganics. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with the following Matters of National Environmental Significance [MNES] receptors:

- White-throated Snapping Turtle (*Elseya albagula*) – Critically endangered; and
- Fitzroy River Turtle (*Rheodytes leukops*) – Vulnerable.

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Attachment 1 Risk Assessment Dossier

CALCIUM CARBIDE

This dossier on calcium carbide presents the most critical studies pertinent to the risk assessment of calcium carbide in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. Most of the information presented in this dossier was obtained from the ECHA database which provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Calcium carbide was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Calcium carbide was assessed as a tier 2 chemical for acute toxicity. Therefore, calcium carbide is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

During a carbide lag test, calcium carbide reacts with water in the drilling fluid rapidly producing calcium hydroxide and acetylene gas. Acetylene is commonly used as a tracer gas for this purpose. It circulates with the drilling fluid until it reaches the surface, where it is detected and captured at the gas trap.

Decomposition product calcium hydroxide is an inorganic compound. It is partially soluble in water, dissociating into calcium (Ca^{2+}) and hydroxyl (OH^-) ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues.

Decomposition product acetylene is a flammable, colourless, gas that is soluble in water. As acetylene is a gas at standard temperature and pressure, biodegradation is not considered relevant. It is not expected to bioaccumulate and has a low potential to adsorb to soil or suspended sediments. Volatilisation is expected to be an important fate process.

Calcium carbide and its decomposition products have low acute toxicity by oral, dermal, and inhalation routes of exposure. It is a skin and eye irritant but does not have sensitising properties. Several epidemiological studies have identified decomposition product calcium hydroxide/calcium oxide as a respiratory irritant. Any systemic effects of calcium carbide are considered to be negligible at normal occupational exposures. Calcium carbide and its decomposition products are not genotoxic or carcinogenic and do not exhibit developmental or reproductive toxicity. Calcium carbide is of moderate toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Calcium ethynediide

CAS RN: 75-20-7

Molecular formula: C_2Ca

Molecular weight: 64.1 g/mol

Synonyms: Calcium carbide; calcium acetylide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Calcium Carbide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Black solid with garlic-like odour	2	ECHA
Melting Point	2300 °C @ 101.3 kPa	2	ECHA
Boiling Point	Not determined, is a solid which melts above 300 °C	-	ECHA
Density	2220 kg/m^3 @ 20 °C	2	ECHA
Vapour Pressure	*	-	-
Partition Coefficient (log K_{ow})	*	-	-
Water Solubility	1.2 g/L @ 20 °C (pH 7)*	2	ECHA

*Due to the rapid decomposition, water solubility, vapour pressure and the log K_{ow} of calcium carbide itself cannot be determined. Solubility of 1.2 g/L is given based on the decomposition products calcium hydroxide and acetylene.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for Calcium Carbide.

NICNAS has assessed calcium carbide in an IMAP Tier 1 assessment, and it was concluded that this chemical poses no unreasonable risk to the human health [1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=75-20-7

5 ENVIRONMENTAL FATE SUMMARY

In contact with water, calcium carbide instantly decomposes hydrolytically, yielding acetylene gas (CAS No. 74-86-2) and calcium hydroxide (CAS No. 1305-62-0). Separate dossiers have been prepared for both of these decomposition products. The hydrolysis half-life for calcium carbide is less than 1 minute. (ECHA). [Kl. Score = 2].

Decomposition product calcium hydroxide is an inorganic compound. It is partially soluble in water, dissociating into calcium (Ca^{2+}) and hydroxyl (OH^-) ions; both are ubiquitous in the environment. The ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues.

Decomposition product acetylene is a flammable, colourless, gas that is soluble in water. As acetylene is a gas at standard temperature and pressure, biodegradation is not considered relevant. It is not expected to bioaccumulate and has a low potential to adsorb to soil or suspended sediments. Volatilisation is expected to be an important fate process.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Calcium carbide and its decomposition products have low acute toxicity by oral, dermal, and inhalation routes of exposure. It is a skin and eye irritant but does not have sensitising properties. Several epidemiological studies have identified decomposition product calcium hydroxide/calcium oxide as a respiratory irritant. Any systemic effects of calcium carbide are considered to be negligible at normal occupational exposures. Calcium carbide and its decomposition products are not genotoxic or carcinogenic and do not exhibit developmental or reproductive toxicity.

B. Toxicokinetics

Studies of the pharmacokinetics (i.e adsorption, distribution, metabolism, and excretion) of calcium carbide are limited. A radiolabelled metabolism study in rats fed by oral gavage at a dose of 30 mg/kg/bw/day for 12 days showed that 99% of calcium carbide is resorbed into the bones with 1.2% of the dose being excreted in the urine (ECHA) [KI. Score =2].

For humans, calcium is an important component of a healthy diet as the mineral is necessary for life. Calcium has particular importance in cell physiology, as Ca^{2+} transport from and into the cytoplasm acts as a signal for numerous cellular processes. Moreover, calcium is stored in bones and teeth of humans and animals and is an integral part of mollusc shells. Thus, calcium is the most abundant metal by mass in many animals. In humans, approximately 99 % of the body's calcium is stored in the bones and teeth, while the rest is important for the functioning of processes like exocytosis, neurotransmitter release or muscle contraction, with special importance for the heart muscle. Calcium levels in blood serum are subject to homoeostatic regulation. However, long-term calcium deficiency may cause rickets and impairment of blood clotting as well as osteoporosis in menopausal women. While a lifelong deficit can affect bone and tooth formation hypercalcaemia (elevated levels of calcium in the blood), impaired kidney function including kidney stone formation and decreased absorption of other minerals may be caused by over-retention of calcium. Moreover, the following potential adverse effects of excessive calcium intake have been proposed: the milk-alkali syndrome (MAS), vascular calcification, increased risk of cardiovascular disease and increased risk of prostate

cancer. In 2003, the Upper Intake Level (UL) was thus set at 2,500 mg calcium/day for adults and for pregnant and lactating women by the Scientific Committee on Food (SCF). (ECHA).

C. Acute Toxicity

There are no acute toxicity studies on calcium carbide. In aqueous solution, calcium carbide rapidly decomposes into calcium hydroxide and acetylene. Acute toxicity studies on the decomposition products are discussed within this section.

In an OECD Guideline 425 (Acute Oral Toxicity: Up-and-Down Procedure) study, the oral LD_{50} value for calcium hydroxide in Wistar female rats was determined to be > 2000 mg/kg/bw/day after 14 days (ECHA) [KI.Score =2].

In an OECD Guideline 402 (Acute Dermal Toxicity) and an EU Method B.3 study, the dermal LD_{50} value for calcium dihydroxide in New Zealand White male and female rabbits was determined to be > 2500 mg/kg/bw/day after 24 hours of exposure and 14 days of observation (ECHA) [KI.Score=2]. Moderate irritation including redness and scabbing was observed.

A LC_0 value of 160500 mg/m^3 air was determined for acetylene after 4 hours of whole-body exposure in Sprague-Dawley rats (ECHA) [KI.Score =2].

D. Irritation

Skin

In an OECD Guideline 404 (Acute Dermal Irritation/Corrosion) study, calcium hydroxide was found to be irritating (erythema and slight edema formation) to Himalayan rabbits with fully reversible effects (ECHA) [KI. Score =2).

In a semiocclusive OECD 404(Acute Dermal Irritation/Corrosion) study, no dermal irritation was observed in New Zealand rabbits after exposure to calcium hydroxide (ECHA) [KI. Score =2). An acid/alkaline reserve *in vitro* method showed that calcium carbide is estimated to be a dermal irritant based on alkali reserve of 14.1 (ECHA) [KI.Score=1].

Eyes

As per OECD Guideline 405 (Acute Eye Irritation/ Corrosion), calcium hydroxide is considered irritating to the eyes of New Zealand white rabbits with irreversible effects to the eye (ECHA) [KI.Score=2].

Respiratory

Potential respiratory irritation of calcium hydroxide and calcium oxide has been assessed in several epidemiological studies and studies in volunteers. Cain et al. (2008) investigated the airway effects of 2.5 mg/m³ CaO in 6 male and 6 female volunteers, who were exposed for 45 min. The maximum effect was reached about 30 min after initiation of exposure, followed by adaptation. The authors interpreted their results as “the highest levels studied here lay at the edge of where people would agree that feel in the nose becomes irritating about 17–18 % carbon dioxide”. Thus, the 2.5 mg/m³ level can be considered at the lowest observed adverse effect level (LOAEL). Because 1 and 2 mg/m³

calcium oxide gave rise to an equivalent effect in a prior 2004 study by the author and for calcium oxide, irritating chemesthesis is considered to start at concentrations below physiologically adverse responses. Thus, 2 mg/m³ is considered to be a protective value when used as occupational exposure limit. (ECHA) [Kl. Score = 2].

E. Sensitisation

There are no adequate studies available to evaluate the sensitisation potential of calcium carbide. However, a weight of evidence approach was taken to determine that calcium carbide and its decomposition products do not have sensitising properties (ECHA).

There are no adequate respiratory sensitisation studies available for calcium carbide and its decomposition products.

F. Repeated Dose Toxicity

In aqueous solution, calcium carbide rapidly decomposes into calcium hydroxide and acetylene. Calcium hydroxide dissociates into calcium and hydroxyl ions. As hydroxyl ions are readily buffered in biological tissue, only calcium ions and gaseous acetylene need to be assessed for systemic adverse effects. Calcium is the most abundant mineral in the human body and part of the normal diet (approx 700 mg/day; ECHA). The second decomposition product, acetylene, has been used for over 100 years as an anaesthetic and as an industrial chemical, and few complications of using this gas have surfaced (ECHA).

Oral

In an OECD Guideline 408 (Repeated Dose 90-Day Oral Toxicity Study in Rodents, calcium (as calcium lactate, a food additive) was added to the feed and water given to male and female Fischer 344/DuCrj rats for a maximum of 20 weeks. No severe toxicological findings at any of the administered doses, drinking water:5, 2.5, 1.25, 0.6, and 0.3 and blended feed: 0, 5, 10, 20, and 30%, were observed therefore the no observed adverse effect level (NOAEL) was set at 1840 mg/kg/bw/day for female rats (ECHA) [KI.Score=2].

Inhalation

Rats were administered acetylene via daily 1- hour whole body inhalation exposure for up to 93 days at the following doses 0 and 25,000 parts per million (ppm). Given the fact that no acetylene related effects or organ toxicity was observed the inhalation no observed effect concentration (NOEC) was set at 25,000 ppm for gross pathology (ECHA)[KI.Score=2].

Respiratory irritation of calcium oxide/hydroxide has been assessed in several studies in volunteers and in occupational settings. Any systemic effects of calcium carbide are considered to be negligible at normal occupational exposures. The calcium fraction in calcium carbide is 63 %. Assuming an exposure level of 1-5 mg/m³ and an air volume of 10 m³ inhaled during an 8-hour workday, this results in an inhaled dose of 6.3-31.5 mg calcium per day. Thus, occupational exposures make a negligible contribution to the daily systemic calcium uptake as the Tolerable Upper Intake Level for calcium is 2500 mg/day, and daily intake of calcium from the diet is estimated at 683-753 mg/day (ECHA).

Dermal

There are no adequate or reliable studies available for calcium carbide or its decomposition products.

G. Genotoxicity

In Vitro Studies

The results of the *in vitro* genotoxicity studies on calcium carbide decomposition products (calcium hydroxide and acetylene) are presented in Table 3.

Table 3 *In Vitro* Genotoxicity Studies on Calcium Carbide decomposition products

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Mammalian cell gene mutation (Chinese hamster ovary, CHO) Test substance: Calcium hydroxide	-	-	2	ECHA
Mammalian cell gene mutation (Mouse lymphoma L5178Y cells) Test substance: Acetylene	-	-	1	ECHA
Chromosome aberration study (mouse lymphoma L5178Y cells and human fibroblast cells) Test substance: Calcium hydroxide	-	-	2	ECHA
Chromosome aberration study in mammalian cells (lymphocytes: human peripheral lymphocytes) Test substance: Calcium hydroxide	-	-	2	ECHA
Gene mutation study in mammalian cells (cultured human dental pulp cells, D824) Test substance: Calcium hydroxide	-	-	2	ECHA
Gene mutation study in bacteria (S. typhimurium: TA97, TA98, and TA100) Test substance: Acetylene	-	-	2	ECHA

*+, positive; -, negative

In Vivo Studies

In an OECD guideline 474 (Mammalian Erythrocyte Micronucleus Test) study, calcium oxide was painted daily on the cheeks of five Syrian golden hamster for five days. There was no difference in micronucleated cells for the control group when compared to the treated animals (ECHA) [KI.Score=2].

H. Carcinogenicity

Oral

In an OECD Guideline 451 (Carcinogenicity Study), 50 male and 50 female Fischer 344 rats were exposed to calcium (as calcium lactate) in their drinking water at 0, 2.5, and 5% for two years. No significant dose-related increase in the incidences of tumours in any organ or tissue was found. The results indicated that calcium lactate is not carcinogenic in F344 rats (ECHA) [KI.Score=2].

Inhalation

In an OECD Guideline 451 (Carcinogenicity Study), 30 male and 30 female Wistar rats and NMRI mice were exposed to acetylene gas vapours for 6h per day or 1 to 2 days a week at a dose of 21.1 mg/m^3 air for 18 months. In the study, acetylene was used as negative control in a carcinogenicity study of dichloroacetylene. A NOEC of 21.2 ppm was established for male and female mice. (ECHA) [KI.Score=2].

I. Reproductive Toxicity

In a multi-generation reproduction study, male and female Swiss mice were fed calcium carbonate orally at dose levels of 0, 5000, 10,000, and 20,000 mg/kg or 2500, 700, and 1400 calcium mg/kg/day. A NOAEL could not be established for the first litter, nor the 2 subsequent litters observed due a lack of adequate experimental information (ECHA) [KI.Score=2].

J. Developmental Toxicity

Oral

Female CD/VAF Plus rats were fed 0.5, 0.75, 1.00, and 1.25% calcium carbonate six weeks before mating, throughout mating, and for 20 days during gestation. There was no evidence of reproductive toxicity observed in the rats so a NOAEL of 1.25 mg/kg/day was established for fetuses and a NOAEL of 227.5 mg/kg/day was established for maternal toxicity (ECHA) [KI.Score=2].

In an OECD Guideline 414 (Prenatal Developmental Toxicity Study), CD-1 mice and Wistar rats received calcium oxide by oral gavage doses of 4.4-440 mg/kg (mice) and 6.8-680 mg/kg (rats) during gestational days 6-15 for 10 consecutive days. There was no evidence of maternal or developmental toxicity therefore both the maternal and developmental NOAEL was determined to be 440 mg/kg for mice and 680 mg/kg rats (ECHA) [KI.Score=2].

Inhalation

No adequate and reliable studies available.

Dermal

No adequate and reliable studies available.

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for calcium carbide follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2021).

Non-Cancer

An oral reference dose was not derived for calcium carbide. The toxicity of calcium carbide is driven by local effects to the lung (respiratory irritation).

The Australian Drinking Water Guidelines doesn't have a limit on health or aesthetics for calcium. The Australian drinking water guideline value for hardness (as calcium carbonate) (200 mg/L) and pH (6.5 to 8.5) may be applicable (ADWG, 2021). Both values are based on aesthetic effects.

Cancer

There was no evidence of carcinogenicity in rat and mouse chronic studies conducted on decomposition product acetylene or read-across substance calcium lactate. Thus, a cancer reference value was not derived.

L. Human Health Hazard Assessment of Physico-Chemical Properties

Calcium Carbide does exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Calcium carbide is of moderate toxicity concern to aquatic organisms based on acute toxicity studies.

B. Aquatic Toxicity

Calcium carbide instantly decomposes hydrolytically upon contact with water/moisture, yielding calcium hydroxide and acetylene. Studies on the acute toxicity to aquatic invertebrates, algae and fish are available that were conducted with technical calcium carbide. Therefore, effects reported in these studies can be attributed to the entirety of the decomposition products of technical calcium carbide, i.e., calcium hydroxide and acetylene, including any impurities of the technical material (ECHA).

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on Calcium carbide.

Table 4 Acute Aquatic Toxicity Studies on Calcium Carbide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss (Rainbow Trout)	96-hour LC_{50}	>50	2	ECHA
Daphnia magna	48-hour EC_{50}	4.62	2	ECHA
Scenedesmus subspicatus (Green Algae)	72-hour EC_{50}	46.5 (growth rate) 12 (biomass)	2	ECHA

Chronic Studies

No adequate studies are available.

C. Terrestrial Toxicity

No adequate studies are available.

D. Calculation of PNEC

The PNEC calculations for calcium carbide follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute $E(L)C_{50}$ values are available for fish (>50 mg/L), invertebrates (4.62 mg/L), and algae (12 mg/L). Results from chronic studies are not available for any of the three trophic levels. On the basis that the data consists of only acute studies for three trophic levels, an assessment factor of 1000 has been applied to the lowest reported $E(L)C_{50}$ value of 4.62 mg/L. The $PNEC_{water}$ is 0.0046 mg/L.

PNEC sediment

No reliable experimental toxicity data on sediment organisms are available. Calcium carbide decomposes rapidly in contact with moisture, forming acetylene and calcium hydroxide. Acetylene, as a gas, will not present in the aquatic environment. In sediment-water systems, calcium oxide will react and release calcium ions and hydroxyl ions. Calcium and hydroxyl ions are ubiquitous in the environment and are found naturally in sediment. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as calcium. Therefore, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. As a result, the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No reliable experimental toxicity data on terrestrial organisms are available. Calcium carbide decomposes rapidly in contact with moisture, forming acetylene and calcium hydroxide. Acetylene, as a gas, will not present in the terrestrial environment. In soil, calcium oxide will react and release calcium ions and hydroxyl ions. Calcium and hydroxyl ions are ubiquitous in the environment and are

found naturally in soil. Calcium is an important constituent of most soils and the minerals found in soil are mostly compounds of calcium with other substances. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as calcium. Therefore, the equilibrium partitioning method cannot be used to calculate the $PNEC_{soil}$.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The biodegradation endpoint is not relevant for calcium carbide. As such calcium carbide does not meet the screening criteria for persistence.

Calcium carbide is not expected to bioaccumulate. In contact with water, calcium carbide instantly decomposes hydrolytically, yielding acetylene gas and calcium hydroxide. Neither decomposition product is expected to bioaccumulate. Thus, calcium carbide does not meet the screening criteria for bioaccumulation.

No chronic aquatic toxicity data exist on calcium carbide; however, the acute EC_{50} values are >1 mg/L in fish, invertebrates and algae. Therefore, calcium carbide does not meet the screening criteria for toxicity.

Therefore, calcium carbide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for calcium carbide.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Calcium Carbide	75-20-7	Not a PBT	No	No	NA	No	No	No	2	No Data	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
CHO	Chinese hamster ovary
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal

IMAP	Inventory Multitiered Assessment and Prioritisation Program
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOEC	No Observed Effect Concentration
NOAEL	no observed adverse effect level
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
TG	Test Guideline

Qualitative Tier 2 Assessment

Chlorous Acid, Sodium Salt

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Chlorous acid, sodium salt is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Chlorous acid, sodium salt	7758-19-2	Breaker	0.0221%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no carcinogenicity studies on chlorous acid, sodium salt, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline value is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Chlorous Acid, Sodium Salt (CAS No. 7758-19-2)	Two-Generation Reproductive Study	Average time to preputial separation	4	1000	0.004	0.014

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil were not calculated. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Chlorous Acid, Sodium Salt (CAS No. 7758-19-2)	*Peudokirchneriella subcapitata*	1	1000	0.001

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Chlorous acid, sodium salt in its dry form is a strong oxidizer. The molecular structure for chlorous acid, sodium salt is presented in **Figure 1**.

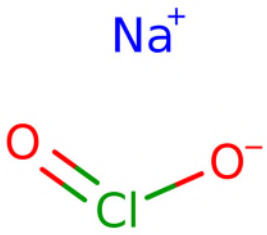

Figure 1 Molecular Structure of Chlorous Acid, Sodium Salt[2]

Chlorous acid, sodium salt readily dissociates in aqueous solutions to the sodium (Na^+) and chlorite (ClO_2^-) ion. Chlorite will ultimately degrade to chloride (Cl^-) ions. Both sodium and chloride ions are ubiquitous in the environment. Biodegradation is not applicable to these inorganic ions. Neither sodium chlorite nor its dissociated ions are expected to adsorb to soil or sediment, or bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) a1sessment for chlorous acid, sodium salt is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

Chlorous acid, sodium salt (sodium chlorite) in solution is moderately-to-highly toxic by the oral route, but has low acute toxicity by the dermal route. It is corrosive the skin and eyes. It is not a skin sensitiser. The critical effect seen in rodents given repeated oral administration of sodium chlorite is hemolytic anemia. Sodium chlorite was not mutagenic in a bacterial reverse mutation (Ames) test; however, chlorine dioxide (which breaks down to chlorite) was mutagenic in the mouse lymphoma assay in the absence and presence of metabolic activation. In vivo genotoxicity studies on sodium chlorite were generally negative. No reproductive toxicity was seen in male or female rats given sodium chlorite in drinking water. There was, however, an effect on post-natal development in pups from the first generation; the effect was not seen in the pups from the second generation. There was no developmental toxicity in pregnant female rabbits given sodium chlorite in drinking water.

In a two-generation reproductive toxicity study conducted in rats, a no observed adverse effect level (NOAEL) of 4 mg/kg-day was established based on increased average time to preputial separation in F2 male pups. This NOAEL was used for determining the oral RfD and the drinking water guideline value (0.014 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

As noted earlier, chlorous acid, sodium salt readily dissociates in aqueous solutions to the sodium (Na^+) and chlorite (ClO_2^-) ion. Chlorite will ultimately degrade to chloride (Cl^-) ions. Both ions are

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/7758-19-2

ubiquitous in the environment. Residual sodium and chloride ions may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to chlorous acid, sodium salt in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system, where over 95% of the residual sodium and chloride ions would go to the brine pond and not be discharged to the river. In addition, sodium and chloride residual concentrations are consistent with or less than geogenic background concentrations.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, chlorous acid, sodium salt is highly toxic to invertebrates and algae and is moderately toxic to fish.

Residual sodium and chloride ions are ubiquitous in the environment. Biodegradation is not applicable to these inorganic ions. Neither sodium chlorite nor its dissociated ions are expected to adsorb to soil or sediment, or bioaccumulate.

PNECs for chlorous acid, sodium salt are provided in **Table 3**. Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNEC for water (see **Table 3**). No experimental toxicity data on sediment or soil organisms are available. Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics. Therefore, PNECs for sediment and soil could not be calculated using the equilibrium partitioning method. Based on its properties, no adsorption of chlorous acid, sodium salt to sediment or soil is to be expected, and the assessment of these compartments will be covered by the aquatic assessment. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water

quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Residual sodium and chloride ions are ubiquitous in the environment. In addition, residual concentrations are de minimis (< 10 mg/L) and consistent with or less than geogenic background. Further, released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

References

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frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.

Attachment 1 Risk Assessment Dossier

CHLOROUS ACID, SODIUM SALT

This dossier on chlorous acid, sodium salt presents the most critical studies pertinent to the risk assessment of chlorous acid, sodium salt in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Chlorous acid, sodium salt was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Chlorous acid, sodium salt was assessed as a tier 1 chemical for acute toxicity of fish and a tier 3 chemical for acute toxicity of algae based on a single reliable acute toxicity study. No chronic studies were available. Based on its potential for rapid degradation in the environment, it is not expected to pose a substantial toxic concern to environmental receptors. Therefore, chlorous acid, sodium salt is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

The main application of chlorous acid, sodium salt is the generation of chlorine dioxide for bleaching and stripping of textiles, pulp, and paper. It is also used for disinfection of municipal water treatment plants after conversion to chlorine dioxide.

Chlorous acid, sodium salt readily dissociates in aqueous solutions to the sodium (Na^+) and chlorite (ClO_2^-) ion. Chlorite will ultimately degrade to chloride (Cl^-) ions. Both sodium and chloride ions are ubiquitous in the environment. Biodegradation is not applicable to these inorganic ions. Neither sodium chlorite nor its dissociated ions are expected to adsorb to soil or sediment, or bioaccumulate.

Chlorous acid, sodium salt (sodium chlorite) in solution is moderately-to-highly toxic by the oral route, but has low acute toxicity by the dermal route. It is corrosive the skin and eyes, but it is not a skin sensitiser. The critical effect seen in rodents given repeated oral administration of sodium chlorite is hemolytic anemia. Sodium chlorite was not mutagenic in a bacterial reverse mutation (Ames) test; however, chlorine dioxide (which breaks down to chlorite) was mutagenic in the mouse lymphoma assay in the absence and presence of metabolic activation. *In vivo* genotoxicity studies on sodium chlorite were generally negative. No reproductive toxicity was seen in male or female rats given sodium chlorite in drinking water. There was, however, an effect on post-natal development in pups from the first generation; the effect was not seen in the pups from the second generation. There was no developmental toxicity in pregnant female rabbits given sodium chlorite in drinking water. It is highly toxic to invertebrates and algae and is moderately toxic to fish.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium chlorite

CAS RN: 7758-19-2

Molecular formula: $ClHO_2.Na$

Molecular weight: 90.44 g/mol

Synonyms: Chlorous acid, sodium salt; sodium chlorite

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Chlorous Acid, Sodium Salt

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White solid, slightly hydroscopic crystals or flakes. Aqueous solutions are colorless to greenish yellow with a slight chlorine-like odor	2	ECHA
Melting Point	180 – 200°C; decomposes at 200°C (pressure not provided)	2	ECHA
Boiling Point	Not applicable	-	-
Density	2,432 kg/m^3 @ 20°C	1	ECHA
Vapor Pressure	1.1 x 10^{-7} Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	<-2.7	1	ECHA
Water Solubility	Very soluble (572 g/L @ 20°C)	1	ECHA

Chlorous acid, sodium salt in its dry form is a strong oxidizer. Chlorous acid, sodium salt readily dissociates in aqueous solutions to the sodium (Na^+) and chlorite (ClO^{2-}) ion. The chlorite (ClO^{2-}) ion is in equilibrium with chlorous acid ($HClO_2$) in water. The chemical reaction is as follows:

$$ClO^{2-} + H^+ \rightleftharpoons HClO_2$$

At pH values found in environmental media or physiological fluids, the chlorite ion will be the predominant form (pKa of chlorous acid is 1.94). Under acidic conditions, chlorous acid ($HClO_2$) will predominate and will disintegrate to chlorine dioxide (ClO_2). Chlorine dioxide (ClO_2) will degrade further to chlorite (ClO^{2-}), and ultimately the chloride ion (Cl^-) is formed. The proportion of each oxy-chlorine species depends in part on the pH of the solution.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No

conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for chlorous acid, sodium salt.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Chlorous acid, sodium salt readily dissociates in aqueous solutions to the sodium (Na^+) and chlorite (ClO_2^-) ion. Chlorite will ultimately degrade to chloride (Cl^-) ions. Both sodium and chloride ions are ubiquitous in the environment. Biodegradation is not applicable to these inorganic ions. Neither sodium chlorite nor its dissociated ions are expected to adsorb to soil or sediment, or bioaccumulate.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Chlorous acid, sodium salt (sodium chlorite) in solution is moderately-to-highly toxic by the oral route, but has low acute toxicity by the dermal route. It is corrosive the skin and eyes. It is not a skin sensitiser. The critical effect seen in rodents given repeated oral administration of sodium chlorite is hemolytic anemia. Sodium chlorite was not mutagenic in a bacterial reverse mutation (Ames) test; however, chlorine dioxide (which breaks down to chlorite) was mutagenic in the mouse lymphoma assay in the absence and presence of metabolic activation. *In vivo* genotoxicity studies on sodium chlorite were generally negative. No reproductive toxicity was seen in male or female rats given sodium chlorite in drinking water. There was, however, an effect on post-natal development in pups from the first generation; the effect was not seen in the pups from the second generation. There was no developmental toxicity in pregnant female rabbits given sodium chlorite in drinking water.

B. Acute Toxicity

The oral LD_{50} in rats is 284 mg/kg (ECHA) [Kl. score = 1]. The oral LD_{50} in rats of a 31% aqueous solution of chlorous acid, sodium salt is 390 mg/kg (ECHA) [Kl. score = 2).

There are no acute inhalation toxicity studies.

The dermal LD_{50} in rabbits is 134 mg/kg (ECHA) [Kl. score = 1]. The dermal LD_{50} in rabbits of a 31% aqueous solution of chlorous acid, sodium salt is >2,000 mg/kg (ECHA) [Kl. score = 2).

C. Irritation

Application of 0.5 mL of undiluted chlorous acid, sodium salt to the skin of rabbits for 4 hours under occlusive conditions was corrosive (ECHA) [Kl. score = 2]. Application of 0.5 mL of a 34.5% solution of chlorous acid, sodium salt to the skin of rabbits for four hours under semi-occlusive conditions was essentially non-irritating (ECHA) [Kl. score = 1].

Instillation of 0.1 mL of a 31% aqueous solution of chlorous acid, sodium salt to the eyes of rabbits was severely irritating (ECHA) [Kl. score = 2].

D. Sensitization

Chlorous acid, sodium salt was not considered to be a skin sensitiser when tested in a mouse local lymph node assay (ECHA). [Kl. score = 1]

E. Repeated Dose Toxicity

Oral

Male and female Crj:CD(SD) rats were dosed by oral gavage with 0, 10, 25, or 80 mg/kg chlorous acid, sodium salt for 13 weeks. Five animals died during the study: one in the 25 mg/kg group and five in the 80 mg/kg group subsequent to blood sampling. The deaths in the 80 mg/kg group were likely treatment-related; the animals were anemic and blood sampling may have exacerbated this problem, contributing to their death. Clinical signs were noted in the 25 and 80 mg/kg animals, the most notable being salivation. Body weights and feed consumption were similar across all groups. Hematological effects were noted in the 80 mg/kg animals. The group mean erythrocyte count was significantly lower (both sexes). In males, hematocrit and hemoglobin levels were significantly lower, and methemoglobin levels and neutrophils counts were significantly higher than controls. The reticulocyte count was increased, but was not statistically significant. Two of the 80 mg/kg rats that prematurely died had marked changes in these hematological parameters. Morphological changes were also seen in the blood smears of three 80 mg/kg females: these were polychromasia, poikilocytosis, macrocytosis, and neutrophilia. Lymphocyte counts were significantly lower than controls in the 80 mg/kg males, and was likely due to the increased neutrophil count. Where the primary red blood cell parameters (mean erythrocyte count, hemoglobin, and hematocrit) were affected, there were also associated changes in mean cell volume, mean cell hemoglobin, and mean cell hemoglobin concentration. In the 25 mg/kg animals (both sexes) and the 10 mg/kg males, statistical trends highlighted a dose-dependent downward trend for erythrocyte counts. Statistical significance was not confirmed by direct comparison with the control group, and group mean values were within background range. Urine volume was unusually high in four 80 mg/kg females, and urinary specific gravity was reduced. There were no histopathologic changes seen in the kidneys of these animals. Absolute and relative spleen weights were increased in the 80 mg/kg males. Absolute spleen weights were increased in the 10 and 80 mg/kg females; relative spleen weights were increased in the 25 and 80 mg/kg females. Relative adrenal weights were increased in the 80 mg/kg males. Absolute adrenal weights were increased in the 80 mg/kg females; relative adrenal weights were increased in the 25 and 80 mg/kg females. Histopathologic changes indicative of chronic irritation were seen in the stomachs of many of the 80 mg/kg animals and a few of the 25 mg/kg males. Extramedullary hematopoiesis was seen in the spleen of a few 80 mg/kg animals and one animal each in the lower two dose groups. The NOAEL for this study is 10 mg/kg-day (ECHA). [Kl. score = 1]

Male C/J and C57L/L mice were given in their drinking water 0, 0.75, 7.5, or 75 mg/L chlorous acid, sodium salt (0, 0.19, 1.9, or 19 mg/kg-day chlorite ion) for 30 days. There were slight signs of oxidative stress of red blood cells at the high-dose. Glucose-6-phosphate dehydrogenase (G6PD) activity and osmotic fragility were slightly increased. Erythrocytes with irregular shapes were also observed. It was suggested that the primary effect of chlorous acid, sodium salt was a disruption of the erythrocyte cell membrane. However, the glutathione level in the erythrocyte was not affected and there were no associated signs of hemolytic anemia, suggesting that the slight increase in G6PD activity acted as a sufficient compensatory mechanism to limit the oxidative stress. The NOAEL for this study is considered to be 7.5 mg/L chlorous acid, sodium salt or 1.9 mg/kg-day chlorite (Moore and Calabrese, 1980). [Kl. score = 2]

Male C57L/J mice were given chlorous acid, sodium salt in their drinking water for 30, 90, or 180 days. The doses were 0, 3, 15, or 75 mg/L expressed as chlorite ion. The average daily doses were estimated to be: 0, 0.74, 3.57, and 17.23 mg/kg-day for the 30-day period; 0, 0.64, 3.15, and 16.2 mg/kg-day for the 90-day period; and 0, 0.69, 3.71, and 17.11 mg/kg-day for the 180-day period. There were no significant changes in body weight gain, absolute or relative kidney weights, water consumption, or histopathologic changes in the kidney. The NOAELs for this study are: 17.23, 16.20, and 17.11 mg/kg-day for the 30-, 90-, and 180-day exposure periods, respectively (Connor et al., 1985). [Kl. score = 2]

Inhalation

No studies are available.

Dermal

No adequate studies are available.

F. Genotoxicity

In Vitro Studies

Table 3 lists the results of the *in vitro* genotoxicity studies on chlorous acid, sodium salt.

Table 3: *In vitro* Genotoxicity Studies on Chlorous Acid, Sodium Salt

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* TA97, TA102 strains)	-	-	4	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	+**	+**	2	ECHA

*+, positive; -, negative

**Test material: chlorine dioxide (chlorite is a breakdown product)

In Vivo Studies

Male and female CD-1 mice were given by oral gavage a single dose of 0, 0.2, 0.5, or 1 mg/day (0, 10, 25, or 59 mg/kg-day) chlorous acid, sodium salt. Chromosomal aberrations were not increased in bone marrow cells of treated mice compared to those in the controls (Meier et al., 1985; ECHA).

Male and female CD-1 mice were given by oral gavage 0, 0.2, 0.5, or 1 mg/day (0, 10, 25, or 59 mg/kg-day) chlorous acid, sodium salt for five consecutive days. There were no significant differences between treated and control mice in the frequency of micronuclei or chromosomal aberrations in bone marrow cells (Meier et al., 1985; ECHA).

Male ddY mice were given a single intraperitoneal injection of 0, 7.5, 15, 30, or 60 mg/kg chlorous acid, sodium salt. Micronucleated polychromatic erythrocytes were statistically significantly increased at all dose levels. The increase was dose-dependent, but the frequency of micronucleated polychromatic erythrocytes decreased at the highest dose level (Hiyashi et al., 1988; ECHA). [Kl. score = 2]

Male ddY mice were given a single intraperitoneal injection of 0 or 15 mg/kg chlorous acid, sodium salt for four consecutive days. The frequency of micronucleated polychromatic erythrocytes were similar between treated and control mice (Hiyashi et al., 1988; ECHA). [Kl. score = 2]

Male ddY mice were given a single oral dose of 0, 37.5, 75, 150, or 300 mg/kg chlorous acid, sodium salt. There was no significant increases in the frequency of micronucleated polychromatic erythrocytes in the bone marrow of the treated mice compared to the controls (Hiyashi et al., 1988; ECHA). [Kl. score = 2]

G. Carcinogenicity

No studies are available.

H. Reproductive Toxicity

A two-generation reproductive toxicity study has been conducted on chlorous acid, sodium salt. Male and female SD rats were given in their drinking water 0, 35, 70, or 300 ppm chlorous acid, sodium salt. The average daily intakes are: 0, 4, 8, and 30 mg/kg-day for males ; and 0, 5, 10, and 39 mg/kg-day for females. The average daily intakes for chlorite are: 0, 2.9, 6, and 22 mg/kg-day for males; and 0, 4, 7.5, and 29 mg/kg-day for females. During lactation, the drinking water levels were reduced 50% to 17.5, 35, and 150 ppm chlorous acid, sodium salt. Water consumption was reduced in all treated groups. Body weights and feed consumption were reduced in the 70 and 300 ppm groups. There was no evidence of reproductive toxicity at any dose level. In the 300 ppm group, pup weights were reduced at birth and on PND 11 (-14%) compared to the controls. There was a decrease in the percent of the 300 ppm F_{2a} pups with eyes open on PND15 compared to the control group; this effects was not observed for the F_1 or F_{2b} pups. There was a small, but statistically significant, increase in the average time to preputial separation for the 70 and 300 ppm F_1 pups and in the vaginal opening for the 300 ppm F_1 pups. Similar changes were not observed for the F_2-generation pups. All of the high-dose animals exhibited mild methemoglobinemia. Thyroid levels were unaffected by treatment. There was a small decrease in the amplitude of auditory startle responses in the 70 and 300 ppm pups on PND 25; the toxicological significance of this effect is

questionable. The NOAEL for reproductive toxicity is 300 ppm chlorous acid, sodium salt, the highest dose tested. The NOAEL for developmental toxicity is 35 ppm (4 and 5 mg/kg-day chlorous acid, sodium salt for males and females, respectively) based on the increase in the average time to preputial separation in the ≥70 ppm F_1 pups. The NOAELs for hematological effects is 70 ppm (8 and 10 mg/kg-day chlorous acid, sodium salt for males and female, respectively). The NOAEL for neurotoxicity is 300 ppm (30 and 39 mg/kg-day chlorous acid, sodium salt for males and females, respectively) (ECHA) [Kl. = 2].

I. Developmental Toxicity

Pregnant New Zealand White rabbits were given 0, 200, 600, or 1,200 mg/L (0, 12.2, 36.6, or 58.8 mg/kg-day) chlorous acid, sodium salt in their drinking water during GD 7 to PND 19. The animals in the mid- and high-dose groups showed reduced water consumption, along with reduced feed consumption, production of fecal pellets, and body weight gain. There was no evidence of embryotoxicity or teratogenicity at any dose level. The NOAELs for maternal and developmental toxicity are 12.2 and 58.8 mg/kg-day, respectively (ECHA). [Kl. score = 1]

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for chlorous acid, sodium salt follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

The lowest NOAEL values from key toxicity studies on chlorous acid, sodium salt are listed below in Table 4.

Table 4: Lowest NOAEL Values from Key Toxicity Studies on Chlorous Acid, Sodium Salt by the Oral Route

Species/sex	Study Duration	mg/kg-day	Endpoint	Reference
Male/female rats	13 weeks	10	Clinical signs, stomach irritation	ECHA
Male pups	2-generation reproductive	4	- average time to preputial separation	ECHA
Male parental rats	2-generation reproductive	8	Hematological effects	ECHA
Female pregnant rabbits	Developmental (GD 6 to PND 17)	12.2	¯ Body weight gain, feed consumption	ECHA

The lowest NOAEL is 4 mg/kg-day based on increased average time to preputial separation in F_2 male pups from a two-generation reproductive toxicity study (ECHA). The NOAEL of 4 mg/kg-day will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Derivation of an Oral Reference Dose

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 4/(10 x 10 x 1 x 10 x 1) = 4/1000 = 0.004 mg/kg-day

Derivation of a drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.004 x 70 x 0.1)/2 = 0.014 mg/L

For comparison, the Australian drinking water guideline value for chlorite is 0.3 mg/L and the Australian drinking water guideline value for sodium is 180 mg/L based on aesthetics (ADWG, 2011).

Cancer

No carcinogenicity studies were found on chlorous acid, sodium salt. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Chlorous acid, sodium salt in solution does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing Potential

[It should be noted that chlorous acid, sodium salt as a solid is a strong oxidizer.]

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Chlorous acid, sodium salt is highly toxic to invertebrates and algae and is moderately toxic to fish.

A. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on chlorous acid, sodium salt.

Table 3 Acute Aquatic Toxicity Studies on chlorous acid, sodium salt

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-h LC_{50}	149	2	ECHA
Daphnia magna	48-h EC_{50}	<1[1]	2	ECHA
Peudokirchneriella subcapitata	96-h EC_{50}	1	1	ECHA

1 – analysis of raw data from the ECHA database indicates that the substance does not comport with expected dose/response. Therefore, this datum is not recommended for use in tiered classifications.

Chronic Studies

No studies are available.

B. Terrestrial Toxicity

No studies are available.

C. Calculation of PNEC

The PNEC calculations for chlorous acid, sodium salt follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (149 mg/L), invertebrates (<1 mg/L), and plants (1 mg/L). On the basis that the data consists of short-term studies from three trophic levels, an assessment factor of 1,000 has been applied to the EC_{50} value of 1 mg/L for algae. The $PNEC_{water}$ is 0.001 mg/L.

PNEC sediment

No reliable experimental toxicity data on sediment organisms are available. Chlorous acid, sodium salt dissociates completely in water with its environmental distribution is dominated by its high

water solubility. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as chlorous acid, sodium salt. Therefore, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. Based on its properties, no adsorption of chlorous acid, sodium salt to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No reliable experimental toxicity data on terrestrial organisms are available. The environmental distribution of chlorous acid, sodium salt is dominated by its water solubility. Sorption of chlorous acid, sodium salt should probably be regarded as a reversible situation, i.e., the substance is not tightly nor permanently bound. K_{oc} and K_{ow} parameters do not readily apply to inorganics, such as chlorous acid, sodium salt. Therefore, the equilibrium partitioning method cannot be used to calculate the $PNEC_{soil}$. Based on its properties, chlorous acid, sodium salt is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Chlorous acid, sodium salt is an inorganic salt that dissociates completely in water to sodium (Na^+) and chlorite (ClO_2^-) ions. Chlorite will ultimately degrade to chloride (Cl^-) ions. Biodegradation is not applicable to these inorganic ions. For the purposes of this PBT assessment, the persistent criteria is not considered applicable to this inorganic salt.

As an inorganic compound, neither chlorous acid, sodium salt nor its dissociated ions are expected to accumulate. Thus, chlorous acid, sodium salt does not meet the criteria for bioaccumulation.

There are no chronic toxicity studies on chlorous acid, sodium salt. The lowest acute $E(L)C_{50}$ values was at 1 mg/L. Thus, chlorous acid, sodium salt does not meet the screening criteria for toxicity.

The overall conclusion is that chlorous acid, sodium salt is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for chlorous acid, sodium salt .

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Chlorous acid, sodium salt	7758-19-2	Not a PBT	No	No	NA	No	No	No	1 (Fish), 3 (algae)	No data available	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). Data available for D. magna suggesting LC50 <1mg/L uncertain and not considered due to poor dose response characteristics. The substance rapidly degrades in water to less toxic chloride ion.

3 – Tier 2 – Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration

ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand

Qualitative Tier 2 Assessment

Cocamide Diethanolamine

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Amides, coco, N,N-bis(hydroxylethyl) (cocamide diethanolamine or cocamide DEA) is a component in a product (CON DET®) used in the KCL/Polymer Stuck Pipe Mud system. The secondary mud system is used to free stuck pipes and, as a secondary mud, will only be used as required. As a result, these secondary muds are considered insignificant relative to the primary muds due to the considerably reduced volume used (<0.1%) as compared to the other muds.

The purpose and maximum quantity (i.e., in all muds) for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Amides, coco, N,N-bis (hydroxyethyl)	68603-42-9	Anionic Surfactant	NA

[1] Based on maximum of combined muds assessed.
CAS No = Chemical Abstracts Service Number
NA = quantity used varies with severity of loss

The assessment of toxicity of cocamide DEA was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. Toxicological reference values (TRVs) were not derived for this chemical. Refer to **Attachment 1** for the rationale for not deriving an oral reference dose, cancer slope factor or drinking water guideline value.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

The determination of TRVs was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 2 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 3** and **4,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 2 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Amides, coco, N,N-bis (hydroxyethyl) (68603-42-9)	Acute *Daphnia*	2.15	1,000	0.002

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 3 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Amides, coco, N,N-bis (hydroxyethyl) (68603-42-9)	[a]	-	-	0.0024

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Amides, coco, N,N-bis (hydroxyethyl) (68603-42-9)	[a]	-	-	0.0011

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Cocamide DEA is a mixture of diethanolamides of the fatty acids derived from coconut oil, which is composed of approximately 48.2% lauric acid (12:0), 18% myristic acid (14:0), 8.5% palmitic acid (16:0), 8% caprylic acid (8:0), 7% capric acid (10:0), 6% oleic acid (18:1 n-9), 2.3% stearic acid (18:0) and 2% linoleic acid (18:2, n-6) (NTP, 2001). It is a substance of unknown or variable composition, complex reaction products or biological materials (UVCB).

Cocamide DEA is produced by a condensation reaction at a 1:1 or 1:2 molar ratio of a mixture of methyl cocoate, coconut oil, whole coconut acids or stripped coconut fatty acids to diethanolamine or DEA (Elder, 1986). Cocamide DEA can be produced in various grades which differ on the basis of the molar ratio of coconut oil methyl esters and diethanolamine used during their manufacture; the purest product is obtained with a molar ratio of 1:1.

Free DEA has been reported by manufacturers to be at 4.0 - 8.5% (Andersen, 1996); however, the cocamide DEA used in the National Toxicology Program (NTP) studies had DEA levels at approximately 18.2% DEA by weight, as well as alkanolamides of unsaturated acids, and amine salts of the acids, and N-Nitrosodiethanolamine (NDELA) detected at a concentration of 219 parts per billion (ppb) (NTP, 2001). In nine commercial samples of cocamide DEA analysed for DEA, the amount of DEA ranged from 3.2% to 14.0%. The NDELA was not found in any of the samples (Chou, 1998).

Cocamide DEA is inherently biodegradable, and it is not expected to bioaccumulate. The major constituent of cocamide DEA (lauramide DEA) has a low tendency to bind to soil or sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for cocamide DEA is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that cocoamide DEA is not a PBT substance.

Human Health Hazards

The acute toxicity of cocamide DEA is low by the oral and dermal routes. It is moderately irritating to the skin and severely irritating to the eyes. There are no data on its skin sensitising potential.

Repeated dose toxicity studies have been conducted in rats and mice by the dermal route. No systemic toxicity was seen. Cocamide DEA is not a reproductive or developmental toxicant. It is not genotoxic. Lifetime dermal studies on cocamide DEA showed no carcinogenic effects in rats; however, in mice there were increased liver tumours (males and females) and kidney tumours (males). The carcinogenic response is considered to be due to DEA, which is present in cocamide DEA as an impurity. The mouse liver tumours are not considered predictive of a carcinogenic response in humans based on studies which have shown choline deficiency as a mechanism of carcinogenesis.

There are no repeated oral dose toxicity studies on cocamide DEA. There are repeated dermal toxicity studies on cocamide DEA in rats and mice, including 14-week and 2-year studies. However, the lack of dermal absorption data complicates extrapolating the dermal doses used in the 14-week and 2-year studies to equivalent oral doses. Therefore, an oral reference dose (RfD) and drinking water guidance value based on non-cancer effects was not derived for cocamide DEA. **Attachment 1** details the rationale for not deriving an oral RfD or drinking water guideline value.

Cocamide DEA may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to cocamide DEA in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in recovered drilling fluids would be diluted by at least 90% in the water feed pond due to the aggregation with produced water. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, cocamide DEA is inherently biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, cocamide DEA is of moderate toxicity concern to aquatic organisms. Acute toxicity towards fish and aquatic invertebrates is of the same order of magnitude. Chronic studies and terrestrial studies are not available.

Cocamide DEA is inherently, but not readily, biodegradable. The chemical also has a low potential for bioaccumulation.

PNECs for cocamide DEA are provided in **Tables 2 – 4**. Experimental toxicity data on water organisms was available for two trophic levels to calculate PNECs. However, no experimental toxicity data on sediment or soil organisms are available. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of cocamide DEA in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of cocamide DEA in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily to inherently biodegradable, such as cocoamide DEA, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 150 days. This is a conservative assumption as biodegradation studies detailed in the dossier provided in **Attachment 1** indicated greater degradation in a less time (i.e., >50% after 28 days).

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

AMIDES, COCO, N,N-BIS(HYDROXYETHYL)
[COCAMIDE DIETHANOLAMINE]

This dossier on amides, coco, N,N-bis(hydroxylethyl) [cocamide diethanolamine or cocamide DEA] presents the most critical studies pertinent to the risk assessment of cocamide DEA in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the United States Environmental Protection Agency High Production Volume Information System (HPVIS) Chemical Challenge Program and from the U.S. Cosmetic Ingredient Review of cocamide DEA (Elder, 1986; Andersen, 1996; Fiume *et al.*, 2013). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Cocoamide diethanolamine was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Cocoamide diethanolamine was assessed as a tier 2 chemical for acute toxicity. No data were available to categorise the substance for chronic toxicity. Therefore, cocamide diethanolamine is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Amides, C8-18 (even number) and C18-unsatd., N,N-bis(hydroxyethyl), also known as cocamide diethanolamine or cocamide DEA is inherently biodegradable, and it is not expected to bioaccumulate. The major constituent of cocamide DEA (lauramide DEA) has a low tendency to bind to soil or sediment. Cocamide DEA is not toxic by the oral and dermal routes. It is moderately irritating to the skin, but severely irritating to the eyes. There are no data on its skin sensitising potential. Repeated dose toxicity studies have been conducted in rats and mice by the dermal route. Except for skin lesions at the site of application due to irritation, there were no non-cancer target organs identified. Lifetime dermal studies on cocamide DEA showed no carcinogenic effects in rats; in mice, there were increased liver tumours (males and females) and kidney tumours (males). The carcinogenic response is thought to be due, not to cocamide DEA itself, but to diethanolamine present in cocamide DEA as an impurity. Studies on the mode of action of the liver tumours from DEA exposure indicate that these tumours are not predictive of a carcinogenic response in humans. However, the relevance of the mouse kidney tumours to human cancer risk is unclear. Animal studies show that developmental toxicity from cocamide DEA exposure is unlikely. Cocamide DEA is of moderate acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Amides, coco, N,N-bis(hydroxyethyl)
CAS RN: 68603-42-9
Molecular formula: $C_{(7+n)}H_{(15+2n)}NO_3$
Molecular weight: 280 to 290 g/mol

Synonyms: Amides, coco, N,N-bis(hydroxyethyl); N,N-bis(hydroxyethyl)cocamides; N,N-bis(hydroxyethyl)coco fatty acid amides; cocamide DEA; cocamide diethanolamine; coco fatty acid

diethanolamides; coconut DEA; coconut diethanolamides; coconut oil diethanolamides; coconut oil diethanolamine

Cocamide DEA is a mixture of diethanolamides of the fatty acids derived from coconut oil, which is composed of approximately 48.2% lauric acid (12:0), 18% myristic acid (14:0), 8.5% palmitic acid (16:0), 8% caprylic acid (8:0), 7% capric acid (10:0), 6% oleic acid (18:1 n-9), 2.3% stearic acid (18:0) and 2% linoleic acid (18:2, n-6) (NTP, 2001).

Cocamide DEA is produced by a condensation reaction at a 1:1 or 1:2 molar ratio of a mixture of methyl cocoate, coconut oil, whole coconut acids or stripped coconut fatty acids to diethanolamine or DEA (Elder, 1986). Cocamide DEA can be produced in various grades which differ on the basis of the molar ratio of coconut oil methyl esters and diethanolamine used during their manufacture; the purest product is obtained with a molar ratio of 1:1. Free DEA has been reported by manufacturers to be at 4.0 – 8.5% (Andersen, 1996); however, the cocamide DEA used in the National Toxicology Program (NTP) studies had DEA levels at approximately 18.2% DEA by weight, as well as alkanolamides of unsaturated acids, and amine salts of the acids, and N-Nitrosodiethanolamine (NDELA) detected at a concentration of 219 ppb (NTP, 2001). In nine commercial samples of cocamide DEA analysed for DEA, the amount of DEA ranged from 3.2% to 14.0%. The NDELA was not found in any of the samples (Chou, 1998).

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Cocamide DEA

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear viscous liquid	-	Fiume *et al.*, 2013
Melting Point	23 – 35°C (pressure not provided)	-	Fiume *et al.*, 2013
Boiling Point	169-275 °C (pressure not provided)	-	IARC
Density	990 kg/m^3 @ 20 °C	-	IARC
Vapor Pressure	-	-	-
Partition Coefficient (log K_{ow})	3.52 (pH and temperature not provided)	-	IARC
Water Solubility	Soluble		Fiume *et al.*, 2013

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for cocamide DEA.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Cocamide DEA is inherently biodegradable. It is not expected to bioaccumulate. The major constituent of cocamide DEA (lauramide DEA) has a low tendency to bind to soil or sediment.

B. Biodegradation

Cocamide DEA is inherently biodegradable. In a modified closed bottle method, degradation was 51.8% degradation after 28 days (HPVIS). However, in an OECD 301D test, there was 84% and 71% degradation after 28 days with 2 mg/L and 5 mg/L cocamide DEA, respectively (HPVIS).

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental studies are available for cocamide DEA. Using KOCWIN™ in EPISuite™ (USEPA, 2017), the estimated K_{oc} values for various diethanoamides present in cocamide DEA are listed in Table 3.

Table 3 K_{oc} Values for Surrogates of Cocamide DEA

Substance	K_{oc} (MCI estimate) L/kg	K_{oc} (log K_{ow} estimate) L/kg
Capramide DEA	11.9	12.76

Substance	K_{oc} (MCI estimate) L/kg	K_{oc} (log K_{ow} estimate) L/kg
Lauramide DEA	39.53	45.02
Myristamide DEA	131.3	156.8
Palmitamide DEA	436.1	546.4
Stearamide DEA	1448	1904
Linoleamide DEA	1448	1101

As mentioned in the previous section, lauramide DEA constitutes approximately 48.2% of the total composition of cocamide DEA(Fiume *et al.,* 2013). Thus, the K_{oc} value for lauramide DEA of 39.53 will be used for calculating the PNEC values for sediment and soil.

Based on the K_{oc} value of lauramide DEA, cocoamide DEA is expected to have a low potential to bind to soil and would be highly mobile. If released to water, based on the K_{oc} value and its solubility, it would likely preferentially partition to water and not adhere to the suspended solids or sediments.

D. Bioaccumulation

No experimental studies are available for cocamide DEA. Using BCFBAF™ in EPISUITE (USEPA, 2017), the estimated BCF values for the various constituents of cocamide DEA range from approximately 8 to 138. Thus, cocamide DEA is anticipated to have a low potential for bioaccumulation.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of cocamide DEA is low by the oral and dermal routes. It is moderately irritating to the skin and severely irritating to the eyes. There are no data on its skin sensitising potential. Repeated dose toxicity studies have been conducted in rats and mice by the dermal route. With the exception of skin lesions at the site of application from irritation, there were no non-cancer target organs. Lifetime dermal studies on cocamide DEA showed no carcinogenic effects in rats; however in mice, there were increased liver tumours (males and females) and kidney tumours (males). The carcinogenic response is considered to be due to DEA, which is present in cocamide DEA as an impurity. The mouse liver tumours are not considered predictive of a carcinogenic response in humans based on studies which have shown choline deficiency as a mechanism of carcinogenesis. Cocamide DEA is not a developmental toxicant.

B. Acute Toxicity

The oral LD_{50} in rats is >5,000 mg/kg (HPVIS).

The dermal LD_{50} in rabbits is >2,000 mg/kg (HPVIS).

C. Irritation

Application of cocamide DEA (30% in propylene glycol) to the skin of rabbits under occlusive conditions was moderately irritating (Fiume et al., 2013).

In rabbit eye irritation studies, a solutions of >64% cocamide DEA and <29% cocamide DEA were considered severe irritants; whereas, in another study, a solution of cocamide DEA in 30% propylene glycol was considered to be a mild eye irritant (Fiume et al., 2013). An *in vitro* (EpiOcular tissue) model was used to evaluate the eye irritation of a 10% solution of cocamide DEA. The test material was considered to be a non-irritant (Fiume et al., 2013).

D. Sensitisation

No adequate studies are available.

E. Repeated Dose Toxicity

Oral

No studies are available.

Inhalation

No studies are available.

Dermal

Male and female F344 rats were given dermal applications of 0, 25, 50, 100, 200 or 400 mg/kg cocamide DEA for 14 weeks. All mice survived until the end of the study. The ≥200 mg/kg dosed males and females had significantly lower final mean body weights compared to the controls. Clinical signs were limited to skin irritation at the site of application in the ≥100 mg/kg animals. Decreased cholesterol levels were seen in the ≥200 mg/kg males and ≥100 mg/kg females. Triglyceride levels were decreased in the ≥200 mg/kg males. Histopathologic effects were seen in the skin at the site of application and consisted of epidermal hyperplasia, sebaceous gland hyperplasia, chronic active inflammation, parakeratosis and ulcers. The incidences and severities of these skin lesions generally increased with increasing dose in both sexes. The incidences of kidney tubule regeneration in the ≥100 mg/kg females were significantly higher than the controls; the severities were also increased in the ≥200 mg/kg females. The NOAEL for systemic toxicity is 100 and 25 mg/kg-day for males and females, respectively. (NTP, 2001). [Kl. score = 1]

Male and female B6C3F_1 mice were given dermal applications of 0, 50, 100, 200, 400 or 800 mg/kg cocamide DEA for 14 weeks. All mice survived until the end of the study. The were no differences between treated and control animals in body weights and body weight gain. Clinical signs were limited to skin irritation at the site of application in the 800 mg/kg animals. Liver and kidney weights were increased in the 800 mg/kg animals, as well as increased liver weights in the 400 mg/kg females and lung weights in the 800 mg/kg females. Histopathologic effects were seen in the skin at the site of application and consisted of epidermal hyperplasia, sebaceous gland hyperplasia, chronic active inflammation, parakeratosis and ulcers. The incidences and severities of these skin lesions

generally increased with increasing dose in both sexes. The NOAEL for systemic toxicity is 800 mg/kg-day (NTP, 2001). [Kl. score = 1]

Male and female F344/N rats were given dermal applications of 0, 50 or 100 mg/kg cocamide DEA (in ethanol) 5 days/week for 104 weeks. The test material contained 18.2% free DEA by weight (9.1 or 18.2 mg/kg DEA, respectively). Survival rates and body weights were similar between treated and control animals. Clinical signs were limited to skin irritation at the site of application in the 100 mg/kg females. The incidences of chronic nephropathy were similar between treated and control animals; however, the severity of nephropathy increased with increasing doses in females. There were non-neoplastic lesions of the skin at the site of application: epidermal hyperplasia, sebaceous gland hyperplasia, parakeratosis and hyperkeratosis; the severities of these effects increased with increasing dose. The incidences of chronic active inflammation, epithelial hyperplasia, and epithelial ulcer of the forestomach increased with dose in females, and were significantly increased in the 100 mg/kg dose group. The NOAEL for non-neoplastic effects is 100 mg/kg-day, the highest dose tested (NTP, 2001).

Male and female B6C3F_1 mice were given dermal applications of 0, 100 or 200 mg/kg cocamide DEA (in ethanol) 5 days/week for 104 weeks. The test material contained 18.2% free DEA by weight (18.2 or 36.4 mg/kg DEA, respectively). Survival was similar across groups. Mean body weights of the 100 mg/kg females (from week 93) and 200 mg/kg females (from week 77) were lower than the controls. Clinical signs were limited to skin irritation at the site of application in the 200 mg/kg males. The incidences of eosinophilic foci in the ≥100 mg/kg males were increased compared to the controls. In the skin, incidences of epidermal hyperplasia, sebaceous gland hyperplasia, and hyperkeratosis were higher in the ≥100 mg/kg animals (both sexes) than in the controls. The incidences of ulcers in the 200 mg/kg males and inflammation and parakeratosis in the 200 mg/kg females were higher than the controls. The incidences of thyroid gland follicular cell hyperplasia in the ≥100 mg/kg animals (both sexes) were greater than the controls. The LOAEL for non-neoplastic effects is 100 mg/kg-day; a NOAEL was not established (NTP, 2001). [Kl. score = 1]

F. Genotoxicity

In Vitro Studies

The results of the *in vitro* genotoxicity studies on cocamide DEA are presented in Table 4.

Table 4 *In Vitro* Genotoxicity Studies on Cocamide DEA

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	1	NTP, 2001
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	NTP, 2001
Chromosomal aberration (CHO cells)	-	-	1	NTP, 2001
Sister chromatid exchange (CHO cells)	-	-	1	NTP, 2001

*+, positive; -, negative

In vivo Studies

Male and female B6C3F_1 mice were given dermal applications of 0, 50, 100, 200, 400 or 800 mg/kg cocamide DEA, 5 days/week for 14 weeks. Peripheral blood was assessed for micronucleated normochromatic erythrocytes at the end of the 14-week exposure period. Micronuclei were statistically significantly increased in the 800 mg/kg males and females, but not at the lower dose levels (NTP, 2001).

G. Carcinogenicity

Oral

No studies were found.

However, relevant human and animal data on DEA from IARC are summarized in the following section.

Inhalation

No studies are available.

Dermal

Male and female F344/N rats were given dermal applications of 0, 50 or 100 mg/kg cocamide DEA (in ethanol) 5 days/week for 104 weeks. The test material contained 18.2% free DEA by weight (9.1 or 18.2 mg/kg DEA, respectively). There was no significant differences in the incidences of tumours between treated and control animals (NTP, 2001). [Kl. score = 1]

Male and female B6C3F_1 mice were given dermal applications of 0, 100 or 200 mg/kg cocamide DEA (in ethanol) 5 days/week for 104 weeks. The test material contained 18.2% free DEA by weight (18.2 or 36.4 mg/kg DEA, respectively). There was a significantly greater incidence of liver tumours in the exposed mice (both sexes) compared to the controls. The liver tumours included hepatocellular adenoma, hepatocellular carcinoma and hepatoblastoma (males). The incidences of hepatocellular adenoma, hepatocellular carcinoma or hepatoblastoma (combined) in the 200 mg/kg male and the $\geq$100 mg/kg females exceeded the historical control ranges. The incidences of renal tubule adenoma and or renal tubule adenoma or carcinoma (combined) in the 200 mg/kg males were significantly greater than the controls and exceeded the historical control ranges for these tumours. No additional kidney tumours were found in an extended kidney analysis. It was noted by NTP that the increases in neoplasms were associated with the concentrations of free DEA present as a contaminant in the cocamide DEA test material based on other studies that had been conducted on different diethanolamides with differing amounts of free DEA and DEA alone (NTP, 2001). [Kl. score = 1]

H. Carcinogenicity (DEA Studies)

NTP Two-year Carcinogenicity Studies

Male and female F344/N rats were dosed with DEA by dermal application for 104 weeks. For males, the doses were 0, 16, 32 or 64 mg/kg-day; and for females, the doses were 0, 8, 16 or 32 mg/kg-day. There was no difference in survival rates between treated and control animals. Mean body weights were lower in the 64 mg/kg-day males from week 8 to 89 and in the 32 mg/kg-day females from week 97 compared to the control animals. The incidences of tumours were not increased in the treated groups compared to the controls (NTP, 1999).

Male and female $B6C3F_1$ mice were dosed with 0, 40, 80 or 160 mg/kg-day DEA by dermal application for 104 weeks. There was reduced survival in the treated female mice (88%, 66%, 66%, and 46% for the 0, 40, 80 and 160 mg/kg-day groups, respectively). This was attributed to liver tumours. No differences were seen in survival rates in the treated male mice compared to the controls. Mean body weights in the 80 and 160 mg/kg-day males were lower than those in the control animals after week 88. Mean body weights in the treated female mice were lower than those of the controls from week 73 (40 and 80 mg/kg-day) and week 53 (160 mg/kg-day).

The incidence of hepatocellular adenomas and of hepatocellular adenomas and carcinomas (combined) were significantly increased in all male and female dose groups, while the incidences of hepatoblastoma was increased in the mid- and high-dose groups. In the female mice, the incidences of hepatocellular neoplasms were significantly higher in all dosed groups compared to the control. Non-neoplastic lesions were seen only in the liver of all male and female dose groups and consisted of cytoplasmic alteration, characterised by mild to moderate enlargement of centrilobular hepatocytes, and syncytial alteration, characterised by scattered hepatocytes with three or more small nuclei.

The incidence of renal tubule adenomas was also increased in males with a positive trend, but the incidences of carcinoma and hyperplasia did not follow this pattern. A step section evaluation found additional adenomas and hyperplasias in all treated male groups. The combined analysis of single and step sections indicated a dose-related increase in the incidence of renal hyperplasia and renal tubule adenoma or carcinoma (combined), and increase in the incidences of renal tubule adenoma in male mice (NTP, 1999).

IARC Assessment and Conclusions

Human carcinogenicity data

Two cohort studies and two nested case–control studies looked at cancer mortality or incidence among workers using metalworking fluids with ethanolamines as additives, with or without sodium nitrite. Small excesses were observed for cancers at various sites, in particular the stomach, oesophagus and larynx. In most of these studies, only associations with use of soluble oils or synthetic fluids were presented and no results were given specifically in relation to DEA exposure. It is difficult to draw conclusions regarding DEA using data from studies of exposures to these complex mixtures.

Animal carcinogenicity data

DEA was tested for carcinogenicity by dermal application in one study in mice and in one study in rats. In the mouse study, there was a treatment-related increase in the incidences of both hepatocellular adenomas and carcinomas in both males and females, as well as an increase in the incidence of hepatoblastomas in males. There was also a marginal increase of renal tubule adenomas in males. In rats, no treatment-related increase in the incidence of tumours was seen in either males or females. In a Tg.AC transgenic mouse model using similar doses to the first mouse study, there was no treatment-related increase in the incidence of skin tumours after skin application.

The limited data available to the Working Group do not indicate that DEA is genotoxic.

Conclusions

There is inadequate evidence in humans for the carcinogenicity of DEA. There is limited evidence in experimental animals for the carcinogenicity of DEA. DEA is not classifiable as to its carcinogenicity to humans.

Mode of Action for Mouse Liver Tumours in DEA-exposed Mice

Effects of DEA on choline homeostatis

Dietary choline deficiency or deprivation induces liver tumours in rodents (Newberne *et al.*, 1982). In contrast, dietary supplementation of choline with or without methionine reduces the incidence of liver tumours in carcinogen-treated mice (Fullerton *et al.* 1990; Newberne *et al.*, 1990). DEA is structurally similar to ethanolamine and choline, important endogenous precursors for normal membrane structure and function. Choline is also oxidised to betaine, an essential methyl group donor in 1-carbon metabolism. The mechanisms by which choline deficiency is thought to be carcinogenic include enhanced cell proliferation, altered methylation status, and altered signal transduction (Rogers, 1995; Zeisel, 1996; Zeisel and Blustjazn, 1994). The development of intracellular choline deficiency as the mode of action by which DEA cause the mouse liver tumours observed in the NTP bioassay is supported by the following experimental evidence:

1. B6C3F_1 mice dosed dermally with 160 mg/kg DEA, 5 days/week for 2 weeks showed a marked decrease in choline metabolites and S-adenosylmethionine (SAM) levels in their livers similar to animals kept on a choline-devoid diet, indicating the development of choline deficiency. These effects were reversed following a 2-week recovery period (Lehman-McKeeman *et al.*, 2002). A significant reduction in the hepatic levels of choline metabolites, including choline, phosphocholine, and glycerophospho-choline, and SAM levels was also reported by Stott *et al.* (2000) with B6C3F_1 mice dosed in a similar regimen with DEA via dermal and/or oral routes.

2. B6C3F_1 mice have a much lower ability than C57Bl/6 mice to maintain nascent methylation capacity, a characteristic that is believed to contribute to a higher spontaneous liver tumour incidence in B6C3F_1 mice (Counts *et al.*, 1996). In a study by Lehman-McKeeman *et al.*, (2002), choline deficiency, as evidenced by changes in phosphocholine concentrations, was produced in both strains of mice. However, unlike the B6C3F_1 mouse, DEA did not alter SAM concentrations in the C57Bl/6 strain.

3. DEA is incorporated into rat liver phospholipids (Barbee and Hartung, 1979; Mathews *et al.*, 1995) and can alter the biosynthesis of hepatic phosphatidylethanolamine and phosphatidylcholine (PC). In cultured cells, DEA inhibited cellular uptake of choline, decreased PC synthesis, and became incorporated into phospholipid fractions. These *in vitro* effects were prevented by culturing cells in the presence of excess choline (Lehman-McKeeman and Gamsky, 1999).

4. DEA caused morphological transformation in Syrian hamster embryo (SHE) cell transformation assay. However, this response was prevented when SHE cells were cultured in a medium containing excess choline (Lehman-McKeeman and Gamsky, 2000).

5. DNA synthesis was increased in mouse and rat, but not human, hepatocytes incubated with DEA. Incubation of mouse and rat, but not human, hepatocytes in medium containing reduced choline increased DNA synthesis. Mouse and rat hepatocytes incubated in medium with excess choline reduced DEA-induced DNA synthesis to control levels or below (Kamendulis and Klaunig, 2005).

6. DNA hypomethylation in GC-rich promotor regions observed in primary mouse hepatocytes which have been treated with DEA are similar to those caused by choline- deficient medium (Bachman *et al.*, 2006).

In situ formation of N-nitrosodiethanolamine

DEA is a secondary amine and may react with a nitrosating agent under certain conditions to form N-nitrosodiethanolamine. This nitrosoamine has been shown to be mutagenic *in vitro* and cause liver tumours in rats at doses of 2 mg/kg-day and higher (ECETOC, 1990). Rats given high, often toxic, oral bolus doses of DEA and nitrite have shown or inferred to produce N-nitrosodiethanolamine (Preussman *et al.*, 1981; Yamamoto *et al.*, 1995). Studies by Stott *et al.* (2000) showed, however, that mimicking the dosing conditions in the NTP study (160 mg/kg DEA dermally) and drinking water supplemented with 170 ppm sodium nitrite to favour nitrosation did not result in N-nitrosodiethanolamine formation in the gastric contents, blood or urine of mice. The findings of Stott *et al.* (2000) suggest that the mouse liver tumours observed in the NTP bioassay were unlikely due to *in situ* nitrosamine formation.

Relevance to Humans

There are marked species differences in susceptibility to choline deficiency, with rats and mice being far more susceptible than other species including humans (Zeisel and Blusztajn, 1994). Rats and mice have a higher dietary choline requirement than humans in large part because rodents oxidise choline more rapidly than humans (Sidransky and Farber, 1960). DEA was carcinogenic in mice, but not in rats, in the NTP dermal carcinogenicity studies. The fact that DEA was not carcinogenic to rats, a species highly susceptible to choline deficiency, should be an important consideration in the overall evaluation of human cancer risk. DEA is less readily absorbed across rat skin than mouse skin, and the resulting blood and tissue concentrations of DEA are at least three-times lower in rats than in mice at similar dosages (Mathews *et al.*, 1995). Lehman-McKeeman *et al.*, (2002) determined the NOAEL for DEA-induced choline deficiency in mice (based on phosphocholine concentrations) to be 10 mg/kg-day. Thus, there is a critical concentration of DEA that must be reached in order to affect choline homeostatis. In the rats, the lack of a carcinogenic response suggests that it is unlikely that

exposure to DEA reached this concentration or that rats are not as susceptible as mice to the effects of DEA on hepatic choline metabolism. Overall, the results suggest that the hepatocarcinogenic effects of DEA in mice are not predictive of similar susceptibility in other laboratory animals or humans.

I. Reproductive Toxicity

No specific reproductive studies are available.

In the 14-week dermal repeated dose NTP studies in rats and mice (see Section E – Repeated Dose Toxicity), epididymis and testis weights were recorded, spermatids were counted, and epididymal spermatozoa were evaluated for concentration and motility. In females, the estrous cycle stages (% of cycle) and lengths (days) were measured. Values were similar across all groups (NTP, 2001).

J. Developmental Toxicity

Pregnant female rats were dosed by oral gavage with 0, 100, 300 or 1,000 mg/kg cocamide DEA on gestational days (GD) 6 to 15. There were no deaths, and body weights and body weight gain were similar between treated and control dams. Clinical signs (salivation and propulsion of the head) were noted in the ≥100 mg/kg dams 1,000 mg/kg, and were particularly severe in the 1,000 mg/kg dams. There was a significant increase in post-implantation loss and total embryonic death in the ≥100 mg/kg groups. These findings occurred in only one female and thus were considered incidental and not related to substance dosing. Significant retardation in ossification of the sternebrae and skull bones were seen in the ≥300 mg/kg groups. These findings were within the normal range of variation for this strain of rat and thus were considered incidental and not related to substance dosing. The NOAEL for maternal and developmental toxicity is 1,000 mg/kg-day (HPVIS). [Kl. score = 1]

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for cocamide DEA follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

There are no repeated oral dose toxicity studies on cocamide DEA, although a pre-natal rat developmental study conducted by oral gavage showed no maternal or developmental toxicity. However, there are repeated dermal toxicity studies on cocamide DEA in rats and mice, including 14-week and 2-year studies. Apart from non-neoplastic lesions in the skin at the site of application, there were no consistent target organ effects in these dermal studies. In the 14-week study, female rats showed an increased incidence (and a dose-dependent increase in severity) of renal tubular degeneration at all dose levels (≥100 mg/kg); however, this effect was not seen in the 2-year dermal study, which showed increased severity of chronic nephropathy, although the incidence in the treated females was similar to that of the controls. Cocamide DEA is a UVCB substance, and there are no data on the dermal absorption of cocamide DEA, the exception being the impurity DEA. The

lack of dermal absorption data complicates extrapolating the dermal doses used in the 14-week and 2-year studies to equivalent oral doses.

Thus, an oral reference dose (RfD) and drinking water guidance value based on non-cancer effects was not derived for cocamide DEA.

Cancer

Cocamide DEA was not carcinogenic to rats in the 2-year NTP dermal bioassay; but, in the mice, there was an increased incidence of liver tumours in males and females and kidney tumours in males (NTP, 2001). NTP concluded that the carcinogenic effects seen with cocamide DEA was primarily due to the contaminant DEA in the test material, which was at a concentration of 18.2%. The evidence for this conclusion was based on a logistic regression analysis of the pooled liver tumour results from four NTP dermal bioassays (diethanolamine, lauramide DEA, oleamide DEA and cocamide DEA): the fatty acid DEA derivatives varied widely with respect to the amount of free DEA contaminant (NTP, 2001).

As discussed above, the mouse liver tumours from DEA exposure are unlikely to be predictive of the carcinogenic risk to humans based on choline deficiency as a mechanism of carcinogenesis. No such evidence exists, however, for the kidney tumours.

NICNAS conducted a human health tier III assessment on diethanolamine (NICNAS). Regarding the classification for carcinogenicity, NICNAS concluded that "[t]he data on the mode of action are insufficient to conclude that diethanolamine-induced tumours in mice are relevant for humans and, therefore, based on the available information, diethanolamine is not classified for carcinogenicity."

Thus, a cancer reference value for cocamide DEA was not derived.

L. Human Health Hazard Assessment Of Physico-Chemical Properties

Cocamide DEA does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Cocamide DEA is of moderate acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 5 lists the results of acute aquatic toxicity studies conducted on cocamide DEA.

Table 5 Acute Aquatic Toxicity Studies on Cocamide DEA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fish	96-hour LC_{50}	6.7	2	HPVIS
Daphnia magna	24-hour EC_{50}	3.3	2	HPVIS
Daphnia pulex	48-hour LC_{50}	2.15 (Test 1) 2.64 (Test 2)	2	HPVIS

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for cocamide DEA follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for two trophic levels. Acute EC_{50} values are available for fish (6.7 mg/L) and invertebrates (2.15 mg/L). On the basis that the data consists of short-term studies from two trophic levels, an assessment factor of 1,000 has been applied to the lowest reported EC_{50} value of 2.15 mg/L for *Daphnia*. The $PNEC_{water}$ is 0.002 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.0024 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (1.56/1280) \times 1000 \times 0.002$
$= 0.0024$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 1.58/1000 \times 2400]$
$= 1.56\ m^3/m^3$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
= 39.53 x 0.04
= 1.58 L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for cocamide DEA calculated from EPISUITE™ using lauramide DEA as a surrogate is 39.53 L/kg.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default]

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.011 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
= (0.79/1500) x 1000 x 0.002
= 0.0011 mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$Kp_{soil} = K_{oc} \times f_{oc}$
= 39.53 x 0.02
= 0.79 m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for cocamide DEA calculated from EPISUITE™ using lauramide DEA as a surrogate is 39.53 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default]

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Cocamide DEA is inherently, but not readily, biodegradable; it degraded 51.8% in 28 days. Given the considerable amount of degradation in the test, it would not be expected to meet to meet the criteria for persistence.

Based on the estimated BCF values of 8 to 138, cocamide DEA does not meet the screening criteria for bioaccumulation.

The acute EC_{50} values for cocamide DEA are >1 mg/L in fish, invertebrates and algae. Thus, cocamide DEA does not meet the screening criteria for toxicity.

The overall conclusion is that cocamide DEA is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for cocamide DEA.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cocamide DEA	68603-42-9	Not a PBT	No	No	No	No	No	No	2	No data	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	USEPA EPISuite module to estimate bioconcentration and bioaccumulation factors
CHO	Chinese hamster ovary
COC	constituent of concern
DEA	diethanolamine
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
F344	Fischer 344
GC	guanine cytosine
HPV	High Production Volume
HPVIS	High Production Volume Information System
IARC	International Agency for Research on Cancer
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effects level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NDLEA	N-Nitrosodiethanolamine
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effects level
NTP	National Toxicology Program

OECD	Organisation for Economic Co-operation and Development
PBT	persistent, bioaccumulative and toxic
PC	phosphatidylcholine
PNEC	Predicted No Effect Concentration
ppb	parts per billion
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	reference dose
SAM	S-adenosylmethionine
SGG	Synthetic Greenhouse Gases
SHE	Syrian hamster embryo
UVCB	unknown or variable composition, complex reaction products and biological materials
µg/kg	micrograms per kilogram
µg/L	micrograms per litre

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
Amides, coco, N,N-bis (hydroxyethyl)	68603-42-9	3.19E+01	1.50E+02	3.19E+00	2.78E+00	3.19E-02	2.78E-02	6.38E-04	5.55E-04	2.00E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Cocamidopropyl Betaine

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Cocamidopropyl betaine is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Cocamidopropyl betaine	61789-40-0	Surfactant	0.0939%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no carcinogenicity studies on cocamidopropyl betaine, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline value is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Cocamidopropyl Betaine (CAS No. 61789-40-0)	Developmental	Maternal toxicity (reduced body weight, stomach ulcers)	95	300	0.32	1.1

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Cocamidopropyl Betaine (CAS No. 61789-40-0)	*Oncorhynchus mykiss*	0.16	50	0.0032

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Cocamidopropyl Betaine (CAS No. 61789-40-0)	[a]	-	-	0.033

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Cocamidopropyl Betaine (CAS No. 61789-40-0)	[a]	-	-	0.028

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Cocamidopropyl betaine is a mixture of closely related organic compounds derived from coconut oil and dimethylaminoproplamine. Cocamidopropyl betaine is a quaternary ammonium compound. However, cocamidopropyl betaine is a zwitterionic compound, and therefore does not have the severe irritant properties of cationic surfactants.

The molecular structure for cocamidopropyl betaine, is presented in **Figure 1**.

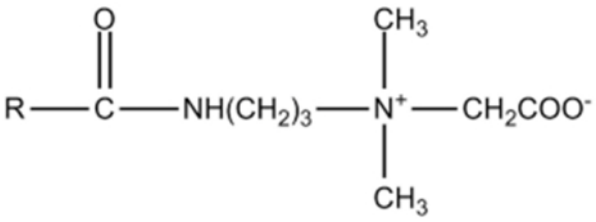

Figure 1 Molecular Structure of Cocamidopropyl Betaine [2]

Cocamidopropyl betaine is readily biodegradable; has a low potential for bioaccumulation; and is expected to have low-to-moderate adsorption to soil and sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for cocamidopropyl betaine is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

The acute toxicity of cocamidopropyl betaine is low-to-moderate by the oral and dermal routes. It is irritating to the skin in humans but is a potentially weak skin sensitiser. The potential for eye irritation is dependent on the concentration of cocamidopropyl betaine. Repeated dose toxicity studies in rats by the oral route have shown that cocamidopropyl betaine is irritating to the gastrointestinal tract, with no indication of any systemic effects up to 300 milligrams per kilogram-day (mg/kg-day). It is not genotoxic; and there was no indication of developmental toxicity in rats given cocamidopropyl betaine by the oral route up to 95 mg/kg-day.

In a developmental toxicity study, dose-related maternal toxic effects (reduced body weights and stomach ulcers) were observed at 990 milligrams per kilogram body weight per day (mg/kg bw/day) and above. Embryotoxic effects (increased numbers of resorptions, decreased number of viable fetuses, decreased fetal body weight) were found only at the maternal toxic dose level of 3300 mg/kg bw/day. The no observed adverse effect level (NOAEL) for maternal toxicity of 330 mg/kg-day (corresponding to 95 mg active substance/kg-day) was used for determining the oral RfD and the drinking water guideline value (1.1 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Cocamidopropyl betaine may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to cocamidopropyl betaine in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface

[2] https://www.industrialchemicals.gov.au/sites/default/files/1-Propanaminium%2C%203-amino-N-%28carboxymethyl%29-N%2CN-dimethyl-%2C%20N-coco%20acyl%20derivatives%2C%20hydroxides%2C%20inner%20salts_Human%20health%20tier%20II%20assessment.pdf

water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, cocamidopropyl betaine is readily biodegradable and does not persist in the environment. In an OECD 301 B test, degradation was 84% and 99% after 7 and 28 days, respectively.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, cocamidopropyl betaine is moderately toxic to aquatic organisms.

Cocamidopropyl betaine is readily biodegradable; has a low potential for bioaccumulation; and is expected to have low-to-moderate adsorption to soil and sediment.

PNECs for cocamidopropyl betaine are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNEC for water (see **Table 3**). There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method (see **Tables 4 and 5**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream

agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of cocamidopropyl betaine in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, first, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as cocoamidopropyl betaine, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days. This is a conservative assumption as biodegradation studies detailed in the dossier provided in **Attachment 1** indicated greater degradation in a less time (i.e., >80% after 7 days). In addition, this chemical is also subject to photolytic degradation (half-life of <10 hours) as well as dissociation in aqueous systems.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Santos, 2013. Dawson River Release Scheme – Environmental Authority Amendment Application – Supporting Information. May 2013.

Attachment 1 Risk Assessment Dossier

COCAMIDOPROPYL BETAINE

This dossier on cocamidopropyl betaine presents the most critical studies pertinent to the risk assessment of cocamidopropyl betaine in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on alkylamidopropyl betaines, which includes cocamidopropyl betaine (OECD, 2006; OECD, 2007), and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Cocamidopropyl betaine was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Cocamidopropyl betaine was assessed as a tier 2 chemical for acute toxicity and a tier 2 chemical for chronic toxicity. Thus, it is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Cocamidopropyl betaine is a mixture of closely related organic compounds derived from coconut oil and dimethylaminoproplamine. Cocamidopropyl betaine is used as a surfactant in many industries including personal care products. It is also used as a surfactant for promoting the formation of gas hydrates. Cocamidopropyl betaine, as an additive, helps to scale-up the gas hydrates formation process.

Cocamidopropyl betaine is readily biodegradable; has a low potential for bioaccumulation; and is expected to have low-to-moderate adsorption to soil and sediment.

The acute toxicity of cocamidopropyl betaine is low-to-moderate by the oral and dermal routes. It is irritating to the skin in humans but is a potentially weak skin sensitiser. The potential for eye irritation is dependent on the concentration of cocamidopropyl betaine. Repeated dose toxicity studies in rats by the oral route have shown that cocamidopropyl betaine is irritating to the gastrointestinal tract, with no indication of any systemic effects up to 300 mg/kg-day. It is not genotoxic; and there was no indication of developmental toxicity in rats given cocamidopropyl betaine by the oral route up to 95 mg/kg-day. The acute and chronic toxicity of cocamidopropyl betaine is of moderate concern to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1-propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-,N-coco acyl derivs., hydroxides, inner salts

CAS RN: 61789-40-0

Molecular formula (mean)* [1]**:** $C_{12.8}H_{39.8}N_2O_3$ [OECD, 2007]

Molecular weight (mean)* [1]**:** ca. 355 g/mol [OECD, 2007]

Synonyms: Cocamidopropyl betaine; 1-propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-,N-coco acyl derivs., hydroxides, inner salts; 1-propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl,N-coco acyl derivs., hydroxides, inner salts; 1-propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-,N-coco acyl derivs., inner salts; cocoamidopropyl betaine; cocoamido propyl betaine; cocoamidopropylbetaine; N-cocamidopropyl-dimethylglycine; coco amide propylbetaine; acetobetain, dimethyl-C12-18-acylamidopropyl-; (N-cocoamidopropyl)-N,N-dimethylglycin, hydroxide, inner salts

3 PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for cocamidopropyl betaine are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Cocamidopropyl Betaine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid	2	ECHA
Melting point	283°C (calculated for C12 fatty acid; QSAR) (pressure not provided)	2	OECD, 2007
Boiling point	651°C for C12 fatty acid (calculated; QSAR) (pressure not provided)	2	OECD, 2007
Density	1,050 – 1,070 kg/m^3@ 20°C	2	OECD, 2007
Vapor pressure	0 Pa @ 25°C (calculated; QSAR)	2	OECD, 2007
Partition coefficient (log	-1.28 to -3.63 @ 25°C*	4	OECD, 2007

[1] *The calculation of the molecular formula and weight is based on the typical alkyl chain length distribution:
C8: 7% (Caprylamidopropyl betaine)
C10: 6% (Capramidopropyl betaine)
C12: 51% (Lauramidopropyl betaine)
C14: 18% (Tetradecylamidopropyl betaine, Myristamidopropyl betaine)
C16: 8% (Palmitamidopropyl betaine)
C18: 10% (Stearamidopropyl betaine)

Property	Value	Klimisch score	Reference
K_{ow})			
Water solubility	0.00162 - 8.769 g/L @ 25^{0}C (calc.) ≥10 g/L @ 25^{o}C (aq. soln, measured)	2	OECD, 2007
Viscosity	38.3259 mPa. S @ 20^{o}C	1	ECHA

*log Kow (C8) = -1.28; log Kow (C10) = -0.30; log Kow (C12) = 0.69; log Kow (C14) = 1.67; log Kow (C16) = 2.65; log Kow (C18) = 3.63.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for cocamidopropyl betaine.

Cocamidopropyl betaine is a quaternary ammonium compound. Quaternary ammonium compounds are listed in the Poisons Standard (Standard for the Uniform Scheduling of Medicines and Poisons (SUSMP, 2014)) in Schedules 5 and 6. However, cocamidopropyl betaine is a zwitterionic compound, and therefore does not have the severe irritant properties of cationic surfactants (NICNAS, 2014), the main group covered by this entry (NICNAS, 2016).

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Cocamidopropyl betaine is readily biodegradable; has a low potential for bioaccumulation; and is expected to have low-to-moderate adsorption to soil and sediment.

B. Biodegradation

Cocamidopropyl betaine is readily biodegradable. In an OECD 301 D test, degradation was 84% after 30 days (ECHA) [Kl. score = 2]. In an OECD 301 E test, degradation was 90% and 100% after 14 and 28 days, respectively (ECHA) [Kl. score = 2]. In an OECD 301 B test, degradation was 84% and 99% after 7 and 28 days, respectively (ECHA) [Kl. score = 2].

If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental studies are available on cocamidopropyl betaine. Using KOCWIN v2.00, the K_{oc} value calculated by the MCI method for cocamidopropyl betaine with a C12 fatty acid side chain is 648 L/kg (ECHA) [Kl. score = 2]. If released to soil, based on this K_{oc} value, the substance has a moderate potential for sorption to soil. If released to water, based on the K_{oc} value and its water solubility, it is expected to also moderately adsorb to suspended solids and sediment.

D. Bioaccumulation

No experimental studies are available on cocamidopropyl betaine. Using the QSAR model BCFBAF v3.01, the bioaccumulation factor (BCF) of cocamidopropyl betaine with a C12 fatty acid chain was estimated to be 70.8 L/kg (ECHA). Thus, the bioaccumulation potential of cocamidopropyl betaine is low (ECHA) [Kl. score = 2].

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of cocamidopropyl betaine is low-to-moderate by the oral and dermal routes. It is irritating to the skin in humans but is a potentially weak skin sensitiser. The potential for eye irritation is dependent on the concentration of cocamidopropyl betaine. Repeated dose toxicity studies in rats by the oral route have shown that cocamidopropyl betaine is irritating to the gastrointestinal tract, with no indication of any systemic effects up to 300 mg/kg-day. It is not genotoxic; and there was no indication of developmental toxicity in rats given cocamidopropyl betaine by the oral route up to 95 mg/kg-day.

B. Acute Toxicity

The oral LD_{50} values for cocamidopropyl betaine are >1,500 mg/kg [Kl. scores = 1].

No acute inhalation studies are available on cocamidopropyl betaine.

The dermal LD_{50} value in rats for cocamidopropyl betaine is >600 mg/kg (OECD, 2007) [Kl. score = 1].

C. Irritation

Application of 0.5 g. of a 30-35% aqueous solution of cocamidopropyl betaine to the skin of rabbits under semi-occlusive conditions were not irritating (OECD, 2007) [Kl. scores = 1].

Skin irritation study was performed on human patients to determine the toxic nature of test chemical. The skin surface water loss (SSWL) values (g/sqmh) at the 1st and 25th minute for the test chemical were 44.7 and 12.1 respectively. Based on these values, test chemical can be considered to be irritating to human skin (ECHA) [Kl. Score = 2].

There are several eye irritation studies conducted on cocamidopropyl betaine in rabbits. A 5-10% solution of cocamidopropyl betaine produced mild to moderate irritation to the eyes of rabbits, which were reversible; solutions containing 15% were irritating to highly irritating; and a 30% aqueous solution was irritating with irreversible damage (OECD, 2006; OECD, 2007 [Kl. scores = 1 and 2].

D. Sensitization

Two independent guinea pig maximization tests have been conducted on cocamidopropyl betaine (OECD, 2006). There was no sensitization response in one test [Kl. score = 2], and the second test gave ambiguous results [Kl. score = 2]. The purity of the cocamidopropyl betaine was not reported.

The sensitizing potential of cocamidopropyl betaine in humans is low. Commercial cocamidopropyl betaine may, however, contain impurities identified as sensitizers (amidoamine and/or 3-dimethylaminopropylamine) which may explain positive results in human patch tests. There is no evidence for a photosensitizing potential. In a guinea pig adjuvant study with less stringent test conditions, cocamidopropyl betaine was not a skin sensitizer (OECD, 2006) [Kl. score = 2]. A modified Draize sensitization test with guinea pigs also showed no sensitization response with cocamidopropyl betaine (OECD, 2006; OECD, 2007) [Kl. score = 2].

A few cases of sensitization in humans have been reported from the use of personal cleansing products containing cocamidopropyl betaine. It is thought that these cases may have been due to impurities of cocamidopropyl betaine, such as amidoamine and DMPA, that could be present in the formulations (OECD, 2006). Nonetheless, cocamidopropyl betaine can be considered to be a potentially weak skin sensitizer.

E. Repeated Dose Toxicity

<u>Oral</u>

Male and female SD rats were dosed by oral gavage with 0, 250, 500 or 1,000 mg/kg of a 30% aqueous solution of cocamidopropyl betaine, 5 days/week for 28 days. The only treatment-related findings were forestomach lesions at the highest dose level, probably as a result of the irritant effect of the test substance. The NOAEL for systemic toxicity in this study is 1,000 mg/kg-day, which corresponds to 300 mg cocamidopropyl betaine/kg-day (OECD, 2006; OECD, 2007) [Kl. score = 2].

Male and female SD rats were dosed by oral gavage with 0, 250, 500 or 1,000 mg/kg of a 30% aqueous solution of cocamidopropyl betaine, 5 days/week for 90 days. The only treatment-related findings were forestomach lesions at the 500 and 1,000 mg/kg dose levels, probably as a result of the irritant effect of the test substance. The NOAEL for systemic toxicity in this study is 1,000 mg/kg- day, which corresponds to 300 mg cocamidopropyl betaine/kg-day (OECD, 2006; OECD, 2007) [Kl. score = 2].

Inhalation

No studies are available.

Dermal

No studies are available.

F. Genotoxicity

In Vitro Studies

The results from in vitro genotoxicity studies on cocamidopropyl betaine are presented in Table 3.

Table 3: *In vitro* Genotoxicity Studies on Cocamidopropyl Betaine

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	1	OECD, 2007
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	1	OECD, 2007
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	1	OECD, 2007
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	4	OECD, 2007

*+, positive; -, negative

In Vivo Studies

Male and female OF1 mice were given intraperitoneal injections of 0, 20, or 200 mg/kg of a 27% solution of cocamidopropyl betaine on two consecutive days. The frequency of micronucleated erythrocytes were similar in the bone marrow cells of the treated mice compared to that in the control mice (OECD, 2006; OECD, 2007) [Kl. score = 2].

G. Carcinogenicity

No studies are available.

H. Reproductive Toxicity

No studies are available. Therefore, the results from the evaluation of reproductive organs from a 90-day repeated dose study with cocamidopropyl betaine in rats were used to assess this endpoint.

In the 90-day toxicity study with a 30 % aqueous solution of cocamidopropyl betaine in rats according to OECD TG 408, no effects on reproductive organ weights (testes, ovaries) and no histopathological changes in reproductive organs (testes, prostate, uterus, ovaries) were found. The NOAEL for reproductive toxicity was at 1000 mg/kg bw/day (OECD, 2007) [Kl. Score = 1].

I. Developmental Toxicity

Pregnant female CD rats were dosed by oral gavage with 0, 330, 990, or 3,300 mg/kg of a 28.9% aqueous solution of cocamidopropyl betaine on GD 5 to 19. The dams in the >990 mg/kg dose groups had reduced body weights and stomach ulcers. Embryotoxic effects (increased numbers of resorptions, decreased number of viable fetuses, decreased fetal body weight) were observed only in the 3,300 mg/kg dose group. The NOAEL for maternal toxicity was 330 mg/kg-day (corresponding to 95 mg cocamidopropyl betaine/kg-day). The NOAEL for developmental toxicity was 990 mg/kg-day, which corresponds to 286 mg cocamidopropyl betaine/kg-day (OECD, 2006; OECD, 2007) [Kl. score = 1].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for cocamidopropyl betaine follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

In a developmental toxicity study, dose-related maternal toxic effects (reduced body weights and stomach ulcers) were observed at 990 mg/kg bw/day and above. Embryotoxic effects (increased numbers of resorptions, decreased number of viable fetuses, decreased fetal body weight) were found only at the maternal toxic dose level of 3300 mg/kg bw/day. The NOAEL for maternal toxicity was 330 mg/kg bw/day (corresponding to 95 mg active substance/kg bw/day) and the NOAEL for developmental toxicity was 990 mg/kg bw/day (corresponding to 286 mg active substance/kg bw). The NOAEL of 95 mg/kg-day will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1

UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 95/(10 x 10 x 1 x 3 x 1) = 95/300 = 0.32 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.32 x 70 x 0.1)/2 = 1.1 mg/L

Cancer

There are no carcinogenicity studies on cocamidopropyl betaine. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Cocamidopropyl betaine does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The acute and chronic toxicity of cocamidopropyl betaine is of moderate concern to aquatic life.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on cocamidopropyl betaine.

Table 4: Acute Aquatic Toxicity Studies on Cocamidopropyl Betaine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hr LC_{50}	2	2	ECHA
Daphnia magna	48-hr EC_{50}	6.4	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50}	48 (growth)	4	ECHA

Chronic Studies

The 28-day NOEC for cocamidopropyl betaine in *Oncorhynchus mykiss* is 0.16 mg/L (ECHA) [Kl. score = 4].

The 21-day NOEC for cocamidopropyl betaine in a Daphnia reproduction test is 0.9 mg/L (ECHA) [Kl. score = 2].

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for cocamidopropyl betaine follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (2 mg/L), invertebrates (6.4 mg/L), and algae (48 mg/L). The NOEC values from chronic studies are available for fish (0.16 mg/L) and invertebrates (0.9 mg/L). On the basis that the data consists of acute studies from three trophic levels and chronic studies from two trophic levels, an assessment factor of 50 has been applied to the lowest reported NOEC value of 0.16 mg/L for fish. The $PNEC_{aquatic}$ is 0.0032 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.033 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (13.24/1280) \times 1000 \times 0.0032$
$= 0.033$ mg/kg ww

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 25.92/1000 \times 2400]$
$= 13.24\ m^3/m^3$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg).
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]
$Kp_{sed} = K_{oc} \times f_{oc}$
$= 648 \times 0.04$
$= 25.92$ L/kg

Where:
K_{oc} = organic carbon normalized distribution coefficient (L/kg). The K_{oc} for cocamidopropyl betaine with a C12 fatty acid side chain calculated from KOCWIN v2.0 using the MCI method is 648 L/kg (ECHA).
F_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.028 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (12.96/1500) \times 1000 \times 0.0032$
$= 0.028$ mg/kg dw

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$Kpsoil = K_{oc} \times f_{oc}$
$= 648 \times 0.02$
$= 12.96\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for cocamidopropyl betaine with a C12 fatty acid side chain calculated from KOCWIN v2.0 using the MCI method is 648 L/kg (ECHA)
F_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU Reach Criteria methodology (DEWHA, 2009; ECHA, 2008).

Cocamidopropyl betaine is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on calculate BCF values of 70.8 L/kg, cocamidopropyl betaine does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on cocamidopropyl betaine is >0.1 mg/L. The acute $E(L)C_{50}$ values for cocamidopropyl betaine in fish, invertebrates, and algae are >1 mg/L. Thus, cocamidopropyl betaine does not meet the screening criteria for toxicity.

The overall conclusion is that cocamidopropyl betaine is not a PBT substance

B. Other Characteristics of Concern

No other characteristics of concern were identified for cocamidopropyl betaine.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cocamidopropyl betaine	61789-40-0	Not a PBT	No	No	No	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
					0	30	0	30	0	30	
Cocamidopropyl betaine	61789-40-0	9.39E+02	1.50E+01	1.25E+02	1.25E+01	3.13E+00	1.25E-01	3.13E-02	2.50E-03	6.26E-04	3.20E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

CTAC

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC) is a component in a product used in the KCl/Polymer Stuck Pipe Mud system. The secondary mud system is used to free stuck pipes and, as a secondary mud, will only be used as required. As a result, these secondary muds are considered insignificant relative to the primary muds due to the considerably reduced volume used (<0.1%) as compared to the other muds.

The purpose and maximum quantity (i.e., in all muds) for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC)	4080-31-3	Biocide	NA

[1] Based on maximum of combined muds assessed.
CAS No = Chemical Abstracts Service Number
NA = quantity used varies with severity of loss

CTAC is an active ingredient in several biocide products. One of these products, DOWICIL 75, is stabilised with sodium bicarbonate (CAS No. 144-55-8). Sodium bicarbonate at ≤ 39% is added to stabilize the active ingredient and in solution will dissociate to the sodium cation and bicarbonate anion. No adverse effects are associated with sodium bicarbonate (see dossier included in **Attachment 1**). Other substances include the following impurities: 1,3-dichloropropene (CAS No. 542-75-6) at <0.25%, dichloromethane (CAS No. 75-09-2) at <0.1%, and hexamethylenetramine (CAS No. 100-97-0) at <5%. These impurities are at *de minimus* levels and for purposes of this assessment are not further evaluated.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on CTAC; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC) (4080-31-3)	90-day rat dietary	Liver	15	1,000	0.015	0.05

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC) (4080-31-3)	Acute Algae	1.5	1,000	0.0015

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC) (4080-31-3)	[a]	-	-	0.0081

[a]Calculated using equilibrium partitioning method.
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC) (4080-31-3)	[a]	-	-	0.0064

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

CTAC is a quaternary ammonium salt. CTAC can be present as a cis- and trans-isomer, depending on the biocide formulation. The molecular structure of CTAC is presented in **Figure 1**.

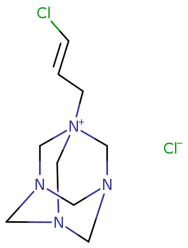

Figure 1 Molecular Structure of CTAC[2]

CTAC is expected to be readily biodegradable, and is not expected to bioaccumulate. It has a medium potential for adsorption to soil or sediments.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for CTAC is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that CTAC is not a PBT substance.

Human Health Hazards

The acute toxicity of CTAC is low-to-moderate by the oral route and low by the dermal route. It is slightly irritating to the skin and eyes; prolonged or repeated contact may cause skin irritation. Skin sensitisation studies on the cis isomer of CTAC have indicated mixed results.

Repeated dose toxicity studies by the oral route have shown the liver to be a target organ; studies conducted by the dermal route showed only irritation at the site of contact and no systemic toxicity. Relatively high oral doses of products containing CTAC have caused birth defects in animal studies; studies conducted by the dermal route have shown no developmental effects. The genotoxicity studies are generally negative. Given the findings from the repeated dose toxicity and genotoxicity studies, there is a low concern for carcinogenicity.

Based on a review of repeated dose and developmental toxicity studies, a TRV was derived for CTAC. The drinking water guideline value derived using the non-carcinogenic oral RfD is 0.05 milligrams per litre (mg/L)(see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

CTAC may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/4080-31-3

There is low potential for human receptors to be exposed to CTAC in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in recovered drilling fluids would be diluted by at least 90% in the water feed pond due to the aggregation with produced water. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, CTAC is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, CTAC is a high acute toxicity concern to algae, but moderately toxic to fish and invertebrates. To birds, it is practically non-toxic on an acute basis and slightly to non-toxic on a subacute dietary basis. CTAC is readily biodegradable and therefore is not persistent in the environment. It does not bioaccumulate.

PNECs for CTAC are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs in water. There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the

release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of CTAC in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of CTAC in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as CTAC, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019.

Department of the Environment and Energy (DoEE). (2017). Exposure draft: Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction. Commonwealth of Australia, available at http://www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual

ECHA. ECHA REACH database: http://echa.europa.eu/information-on-chemicals/registered-substances

frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.

Santos, 2013. Dawson River Release Scheme – Environmental Authority Amendment Application – Supporting Information. May 2013.

Attachment 1 Risk Assessment Dossier

1-(3-CHLOROALLYL)-3,5,7-TRIAZA-1-AZONIAADAMANTANE CHLORIDE (CTAC)

This dossier on 1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC) presents the most critical studies pertinent to the risk assessment of CTAC in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – CTAC is an active ingredient in several biocide products. One of these products, DOWICIL 75, contains CTAC (64%) (CAS 4080-31-3) along with sodium bicarbonate (<39%) (CAS 144-55-8), methenamine (<5%) (CAS 100-97-0), 1,3-dichloropropene (<0.25%) (CAS 542-75-6) and methylene chloride (<0.1%) (CAS 75-09-2). For the purposes of this dossier, methenamine, 1,3-dichloropropene and methylene chloride occur at *de minimus* levels and do not warrant further hazard assessment. A standalone dossier has been developed for sodium bicarbonate wherein it is classified as a Tier 1 chemical. CTAC was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. CTAC was assessed as a tier 2 chemical for acute toxicity. No chronic toxicity data were available to categorize the substance. Therefore, CTAC is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

CTAC is readily biodegradable, and is not expected to bioaccumulate. It has a medium potential for adsorption to soil or sediments. The acute toxicity of CTAC is low-to-moderate by the oral route and low by the dermal route. It is slightly irritating to the skin and eyes; prolonged or repeated contact may cause skin irritation. Although the Dowicil products have tested negative for skin sensitisation in animals and humans, Dowicil 75 contains hexamethylenetetramine, which is a skin sensitiser. Repeated dose toxicity studies by the oral route have shown the liver to be a target organ; studies conducted by the dermal route showed only irritation at the site of contact and no systemic toxicity. The genotoxicity studies are generally negative. Dowicil 75 contains traces of impurities (methylene chloride and 1,3-dichloropropene) known to cause cancer in animal studies. Given the findings from the repeated dose toxicity and genotoxicity studies, there is a low concern for carcinogenicity for CTAC. Relatively high oral doses of Dowicil products containing the same active ingredient as Dowicil 75 (CTAC) have caused birth defects in animal studies; studies conducted by the dermal route have shown no developmental effects. CTAC is of high acute toxicity concern to algae, but moderately toxic to fish and invertebrates. To birds, it is practically non-toxic on an acute basis and slightly to non-toxic on a subacute dietary basis.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride
CAS RN: 4080-31-3
Molecular formula: $C_9H_{16}N_4Cl_2$
Molecular weight: 251.2 g/mol

Synonyms: Methenamine 3-chlorallylochloride; hexamethylenetetramine chloroallyl chloride; 1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride; 3,5,7-triaza-1-azoniatricyclo[3.3.1.13,]decane, 1-(3-chloro-2-propenyl)-chloride; CTAC, DOWICIL™ 75; quaternium-15; CTAC

The active ingredient of DOWICIL 75 is 1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride (CTAC), and it is stabilised with sodium bicarbonate. The composition of the product is shown below in Table 1. Sodium bicarbonate at ≤ 39% is added to stabilize the active ingredient and in solution will dissociate to the sodium cation and bicarbonate anion. No adverse effects are associated with sodium bicarbonate. The other substances are at *de minimus* levels and for purposes of this dossier are not further evaluated.

Table 1 Composition of Dowicil 75 (Dow, 2014)

Component	CAS Number	Composition
CTAC	4080-31-3	64.0%
Sodium bicarbonate	144-55-8	≤39.0%
Methenamine	100-97-0	<5%
1,3-Dichloropropene	542-75-6	≤0.25%
Methylene chloride	75-09-2	<0.1%

There are three Dowicil products: Dowicil 75, Dowicil 150 and Dowicil 200. CTAC is the active ingredient in all three products. CTAC can be present, however, as a cis- and trans-isomer. Dowicil 75 contain both isomers in roughly equal amounts; whereas, Dowicil 150 and 200 contain the cis-isomer (SCCS, 2011). As the CTAC comprises by far the largest percentage of Dowicil 75 components, the following dossier will focus on testing that has been conducted either on the Dowicil 75 product or CTAC.

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 2.

Table 2 Overview of the Physico-chemical Properties of CTAC

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Powder, with a slight amine-like odour	-	USEPA, 1995
Melting Point	178-210°C	-	USEPA, 1995
Density	400 kg/m^3	-	USEPA, 1995
Vapor Pressure	<1.3 x 10^{-5} Pa @ 25°C	-	USEPA, 1995
Partition Coefficient (log K_{ow})	-0.1 (measured) 0.3 (measured)	-	USEPA, 1995 Dow, 2013
Water Solubility	> 100 g/L @ 25°C	-	PubChem

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 3). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for CTAC.

Table 3 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

CTAC is readily biodegradable, and is not expected to bioaccumulate. It has a medium potential for adsorption to soil or sediments.

B. Partitioning

CTAC is 97.8% ionized in moist soil, indicating that this compound will exist almost entirely in cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Because of these cations, volatilization in moist soil surfaces and in water is not expected to be an important fate process (PubChem).

The aqueous hydrolysis half-lives of CTAC (58 ppm concentration, 25 °C) were reported as 1.1, 2.7, and 2.2 days at pH 5, 7, and 9, respectively (PubChem).

C. Biodegradation

Dowicil 75 is readily biodegradable. In an OECD 301A test, there was 75% degradation after 28 days (Dow, 2013). In an OECD 306 test, there was 83-90% degradation after 28 days (Dow, 2013).

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for CTAC. The estimated soil K_{oc} is 320 (Dow, 2013) which indicates a moderate potential for sorption. If released to soil, based on this K_{oc} value along with its ionization properties, CTAC is expected to be moderately mobile.

E. Bioaccumulation

Bioconcentration of CTAC in aquatic organisms is not expected to occur based on a measured log K_{ow} of -0.1 (USEPA, 1995).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of CTAC is low-to-moderate by the oral route and low by the dermal route. It is slightly irritating to the skin and eyes; prolonged or repeated contact may cause skin irritation. Although the Dowicil products have tested negative for skin sensitisation in animals and humans, Dowicil 75 contains hexamethylenetetramine which is a skin sensitiser. Repeated dose toxicity studies by the oral route have shown the liver to be a target organ; studies conducted by the dermal route showed only irritation at the site of contact and no systemic toxicity. The genotoxicity studies are generally negative. Dowicil 75 contains traces of impurities (methylene chloride and 1,3-dichloropropene) known to cause cancer in animal studies. Given the findings from the repeated dose toxicity and genotoxicity studies, there is a low concern for carcinogenicity for CTAC. Relatively high oral doses of Dowicil products containing the same active ingredient as Dowicil 75 (CTAC) have caused birth defects in animal studies; studies conducted by the dermal route have shown no developmental effects.

B. Acute Toxicity

The oral LD_{50} for Dowicil 75 in rats is 1,000 to 2,000 mg/kg; and the dermal LD_{50} in rabbits is >5,000 mg/kg (Dow, 2013).

C. Irritation

The Dowicil 200 (cis-CTAC) is slightly irritating to the skin and eyes of rabbits (SCCS, 2011). However, prolonged or repeated skin contact may cause irritation (see Section E).

D. Sensitisation

Dowicil 200 (cis-CTAC) was not considered to be a skin sensitiser in a guinea pig maximisation test. The induction and challenge doses were a 10% solution in Dowanol DPM/Tween 80 (9:1) (SCCS, 2011).

The Dowicil 200 (cis-CTAC), which was 0.6% in petrolatum, did not induce allergic contact dermatitis in a human repeat insult patch test (HRIPT) (SCCS, 2011). However, in another HRIPT, Dowicil 200 at 1% was considered to be a potential skin sensitiser. There are a number of published studies on the human patch test results for Quaternium-15; these have been reviewed by De Groot et al. (2010).

The Dowicil products contain the impurity hexamethylenetetramine (CAS No. 100-97-0), which is a known skin sensitiser.

E. Repeated Dose Toxicity

Oral

Male and female Sprague Dawley (SD) rats were given in their diet 0, 7.5, 15, 30 or 60 mg/kg Dowicil 100 (cis-/trans-CTAC, 91% purity) for 90 days. There were significantly decreased body weights (up to 20%) and a corresponding decrease in feed consumption in all dose groups (both sexes). Brain weights relative to body weights were significantly increased in all dose groups (both sexes); testis weights relative to body weights were significantly increased in male of all dose groups. Relative liver weights to body weights were increased in the 60 mg/kg animals (both sexes). In the 60 mg/kg males, serum urea nitrogen levels were significantly higher and alkaline phosphatase levels were significantly lower. SGPT levels were significantly lower in the ≥15 mg/kg males. Hepatocellular swelling was seen in some 60 mg/kg males. The NOAEL for this study is considered to be 15 mg/kg-day (SCCS, 2011). [Kl. score = 2]

Inhalation

No studies are available.

Dermal

A modified OECD 422 study was conducted on a cis-/trans-CTAC product (30.9% cis, 32.0% trans). Male and female Crl:CD(SD) rats were given dermal applications of 0, 75, 225 or 750 mg/kg (dose levels have been corrected for purity of cis-/trans-CTAC) for 6 hours/day. Males were dosed for 10 weeks, starting with a 4-week pre-mating period. Females were dosed from 4 weeks prior to mating until the end of lactation. The F_1 offspring were dosed for one week following weaning. The 750 mg/kg group was terminated early on day 17 of the study due to the severity of the skin lesions. There were no treatment-related clinical signs. The 225 mg/kg animals had scaling, erythema, and edema of the skin; these effects were minor in the 75 mg/kg animals. Female final body weights were significantly lower (8.1%) in the 225 mg/kg females; the 225 mg/kg males had lower (5.8%) final body weights that were not statistically significant. The 225 mg/kg males and females had significantly lower feed consumption; for the females, it was significantly reduced throughout the pre-mating period. Haematological parameters were similar between treated and control groups. There was a dose-related change in triglyceride levels, with statistical significance in the 225 mg/kg males. Chloroallylamine, the metabolite of CTAC, was found in the urine of treated rats. Histopathological effects in the parental animals were limited to skin lesions in two 225 mg/kg females. The NOAEL for parental toxicity is 75 mg/kg-day (SCCS, 2011). [Kl. score = 1]

Male and female New Zealand White rabbits were given dermal applications of 0, 50, 200 or 1,000 mg/kg Dowicil 100 (cis-/trans-CTAC; two batches of 94.85% and 90.2% purity) 6 hours/day, 5 days/week for 91 days. There were signs of irritation at the test site, which ranged from slight to severe erythema, edema and scaling, slight fissuring, scabbing and scarring, mainly limited to areas of abrasion from clipping. The onset and degree of skin changes were dose-related. Haematological parameters in treated males were similar to the controls; however, there was an increase in white blood cell count and platelets in the 1,000 mg/kg females. There were no treatment-related changes

in the clinical chemistry. Gross pathological findings and histopathology were limited to the skin at the site of application. The NOAEL for systemic toxicity is 1,000 mg/kg-day (SCCS, 2011).

Male and female mice were given dermal applications of 0, 100, 400 or 1,200 mg/kg Dowicil 100 (cis-/trans-CTAC, 91.3% purity) 6 hours/day for 90 days. There was no indication of systemic toxicity. The NOAEL for systemic toxicity is 1,200 mg/kg-day (SCCS, 2011).

F. Genotoxicity

In Vitro Studies

The results of the *in vitro* genotoxicity studies on CTAC are presented below in Table 4.

Table 4 *In Vitro* Genotoxicity Studies on CTAC

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Mammalian cell gene mutation (CHO cells/HGPRT)	-	+	-	USEPA, 1995; SCCS, 2011
Unscheduled DNA synthesis (rat hepatocytes)	NA	-	-	USEPA, 1995

*+, positive; -, negative; NA, not applicable.

In Vivo Studies

CTAC was negative in mouse micronucleus test. No details were given (USEPA, 1995). Dowicil 200 (cis-CTAC) did not induce micronuclei in the bone marrow cells of male CD-1 mice given up to 2,000 mg/kg as a single oral dose on two consecutive days (SCCS, 2011). Dowicil 150 (cis-CTAC) did not induce unscheduled DNA synthesis (UDS) in male F344 rats given 750 or 1,500 mg/kg as a single oral gavage dose (SCCS, 2011).

G. Carcinogenicity

No studies are available.

H. Reproductive Toxicity

Oral Studies

No studies are available.

Dermal Studies

A modified OECD 22 study was conducted on a cis-/trans-CTAC product (30.9% cis, 32.0% trans). Male and female Crl:CD(SD) Sprague Dawley rats were given dermal applications of 0, 75, 225 or 750 mg/kg (dose levels have been corrected for purity of cis-/trans-CTAC) for 6 hours/day. Males were dosed for 10 weeks, starting with a 4-week pre-mating period. Females were dosed from 4 weeks prior to mating and until the end of lactation. The F_1 offspring were dosed for one week following weaning. The 750 mg/kg group was terminated early on day 17 of the study due to the severity of

the skin lesions. Parental toxicity for this study is described above in the Repeated Dose Toxicity section. Reproductive indices, pup survival and sex ratio were similar across all groups. The 225 mg/kg male and female pup weights tended to decrease (7.5-14.7%) relative to controls throughout the lactation period. On PND 21, the mean female pup weights were statistically significantly lower than the controls. There were no treatment-related clinical signs in the F_1 weanlings, and dermal effects were seen in only one 225 mg/kg male (slight scaling on test days 5 to 7). Body weights of the 225 mg/kg male F_1 offspring were significantly lower than control on test days 4 and 7; the 225 mg/kg female F_1 offspring had lower body weights, but were not statistically significantly different from controls. Feed consumption was significantly lower in the 225 mg/kg males. The NOAEL for reproductive toxicity is 750 mg/kg-day. The NOAEL for post-natal toxicity is 75 mg/kg-day (SCCS, 2011). [Kl. score = 1]

I. Developmental Toxicity

Oral Studies

Pregnant female New Zealand White rabbits were dosed by oral gavage with 0, 2.5, 8 or 25 mg/kg cis-/trans-CTAC product (31.3% cis, 32.5% trans) on gestational days 7-27. Body weight gain and feed consumption were decreased throughout the entire dosing period in the 25 mg/kg does. Foetal body weights and mean gravid uterine weights were also lower in the 25 mg/kg group. The NOAEL for maternal and developmental toxicity is 8 mg/kg-day (SCCS, 2011). [Kl. score = 2]

Pregnant female F344 rats were dosed by oral gavage with 0, 5, 25 or 75 mg/kg Dowicil 200 (cis-CTAC) on gestational days 6 through 15. Body weight and body weight gain were significantly lower in the 75 mg/kg dams. Absolute and relative liver weights were also increased in the 75 mg/kg dams. The 25 mg/kg dams had significantly lower body weights during the first three days of dosing. Food consumption was significantly lower in the 75 mg/kg dams; water consumption was also significantly lower. Feed consumption was also significantly lower in the 25 mg/kg dams during GD 9 through 14. The incidence of resorptions was significantly increased in the 75 mg/kg group, and there was a significant decrease in foetal body weights. The incidence of total major malformation of foetuses was significantly higher in the $\geq$25 mg/kg groups. The majority of the malformed foetuses exhibited anomalies of the eye, microphthalmia or anophthalmia. The NOAEL for maternal and developmental toxicity is 5 mg/kg-day (SCCS, 2011). [Kl. score = 1]

In a repeat study done 23 years later, pregnant female F344 rats were dosed by oral gavage with 0, 25 or 75 mg/kg Dowicil 200 (cis-CTAC) during gestational days 6 through 15. The dams showed similar toxicity as in the previous developmental study on cis-CTAC: decreases in maternal body weight, body weight gains and feed consumption. Foetal body weights were also decreased in the 75 mg/kg dose group. The incidence of microphthalmia and/or anophthalmia was similar to the historical control incidence for F344 rats, and was considerably lower than the incidence of eye defects in the first study. There was no dose-response relationship with respect to these malformations. The study authors concluded that the known propensity of F344 rats for foetal eye defects suggests that the original study findings were likely related to a spontaneously occurring genetic cluster effect, rather than a specific consequence of Dowicil 200 exposure.

Dermal Studies

Pregnant female F344 rats were given dermal applications of 0, 250 or 500 mg/kg CTAC on gestational days 6 to 15. There was no maternal or developmental toxicity. The NOAEL for maternal and developmental toxicity is 500 mg/kg-day (USEPA, 1995).

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for CTAC follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

A 90-day rat dietary study is available on former product Dowicil 100, which can be used to read-across to Dowicil 75 (SCCS, 2011). Both products contain a mixture of cis- and trans-isomer of CTAC. The NOAEL for this study is 15 mg/kg-day, which will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 15/(10 x 10 x 1 x 10 x 1) = 15/1000 = 0.015 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.015 x 70 x 0.1)/2 = 0.05 mg/L

K. Cancer

There are no carcinogenicity studies on the Dowicil products containing either cis-CTAC or cis-/trans-CTAC. Therefore, no cancer reference value was derived.

It should be noted that methylene chloride and 1,3-dichlorpropene are impurities of Dowicil 75. Both substances have been shown to be carcinogenic in laboratory animals.

L. Human Health Hazard Assessment of Physico-Chemical Properties

CTAC does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

CTAC is of high acute toxicity concern to algae, but moderately toxic to fish and invertebrates. To birds, it is practically non-toxic on an acute basis and slightly to non-toxic on a subacute dietary basis.

B. Aquatic Toxicity

Acute Studies

Table 5 lists the results of acute aquatic toxicity studies conducted on CTAC.

Table 5 Acute Aquatic Toxicity Studies on CTAC

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Bluegill	96-h LC_{50}	59	-	ECOTOX
Bluegill	96-h LC_{50}	>148	-	ECOTOX
Fathead minnow	96-h LC_{50}	29	-	ECOTOX
Fathead minnow	96-h LC_{50}	34	-	ECOTOX
Sheepshead minnow	96-h LC_{50}	>122	-	ECOTOX
Rainbow trout	96-h LC_{50}	20.5	-	ECOTOX
Rainbow trout	96-h LC_{50}	>144	-	ECOTOX
Daphnia magna	48-h EC_{50}	27	-	ECOTOX
Daphnia magna	48-h EC_{50}	40	-	ECOTOX

Pseudokrichneriella subcaptitata	EC_{50} NOEC	1.5 (growth rate) 0.243	-	Dow, 2013

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

Avian Species

The oral acute LD_{50} of CTAC to mallard ducks is >2,510 mg/kg (USEPA, 1995). The dietary subacute LC_{50} to bobwhite quail and mallard ducks are 3,223 and >5,620 ppm, respectively (USEPA, 1995).

D. Calculation of PNEC

The PNEC calculations for CTAC follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. The acute EC_{50} values are available for fish (20.5 mg/L), *Daphnia* (27 mg/L), and algae (1.5 mg/L). On the basis that the data consists of short-term results from three trophic levels, an assessment factor of 1,000 has been applied to the lowest reported EC_{50} value of 1.5 mg/L for algae. The $PNEC_{water}$ is 0.0015 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.0081 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$

$= (6.94/1280) \times 1000 \times 0.0015$

$= 0.0081$ mg/kg

Where:

$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)

BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]

$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$

$= 0.8 + [0.2 \times 12.8/1000 \times 2400]$

$= 6.94\ m^3/m^3$

Where:

Kp_{sed} = solid-water partition coefficient (L/kg)

BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
= 320 x 0.04
= 12.8 L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for CTAC is estimated to be 320 L/kg.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default]

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.0064 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
= (6.4/1500) x 1000 x 0.0015
= 0.0064 mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$Kp_{soil} = K_{oc} \times f_{oc}$
= 320 x 0.02
= 6.4 m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for CTAC is estimated to be 320 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default]

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

CTAC is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -0.1, CTAC does not meet the screening criteria for bioaccumulation.

The 96-h NOEC from an algal study on CTAC is >0.1 mg/L. The acute EC_{50} values for CTAC are >1 mg/L in fish, invertebrates and algae. Thus, CTAC does not meet the screening criteria for toxicity.

The overall conclusion is that CTAC is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for CTAC.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
CTAC (64%)	4080-31-3	No	No	No	No	No	No	No	2	No data	2
Sodium bicarbonate (<39%)[4]	144-55-8	No	No	No	No	No	No	No	1	No data	1
Methenamine (<5%)[5]	100-97-0	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1,3-Dichloropropene (<0.25%) [5]	542-75-6	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Methylene chloride (<0.1%) [5]	75-09-2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

4 – Refer to sodium bicarbonate dossier

5 – De minimus level: no further assessment warranted.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
CHO	Chinese hamster ovary
COC	constituent of concern
CTAC	1-(3-chloroallyl)-3,5,7-triaza-1-azoniaadamantane chloride
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
GD	Gestation day
HGPRT	hypoxanthine-guanine phosphoribosyltransferase
HRIPT	human repeat insult patch test
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mm	millimetre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme

NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PND	post natal day
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	reference dose
SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases
SGPT	Serum glutamic pyruvic transaminase
UDS	unscheduled DNA synthesis

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
3,5,7-Triaza-1-azoniatricyclo[3.3.1.13,7]decane,1-(3-chloro-2-propenyl)- , chloride (CTAC)	4080-31-3	3.20E-01	1.50E+01	3.20E-02	8.00E-03	3.20E-04	8.00E-05	6.40E-06	1.60E-06	1.50E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Alcohols, C11-14-iso, C13-rich ethoxylated

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Alcohols, C11-14-iso, C13-rich ethoxylated (hereafter referred to as ethoxylated branched C13 alcohol) is a component in a drilling and completions product used as a shale inhibitor. The purpose and maximum quantity for this chemical is summarised in **Table 1**.

Table 1 Completions Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Ethoxylated Branched C13 Alcohol	78330-21-9	Shale Inhibitor	NA

[1] Based on maximum of combined muds assessed
CAS No = Chemical Abstracts Service Number
NA = Not available

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no adequate or reliable carcinogenic studies available for ethoxylated branched C13 alcohol; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in **Attachment 1**. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Ethoxylated Branched C13 Alcohol (78330-21-9)	2-yr dietary study in rats	Increased organ weights	50	100	0.5	1.8

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Ethoxylated Branched C13 Alcohol (78330-21-9)	-	-	-	0.14[a]

[a] $PNEC_{water}$ for ethoxylated C12-C16 alcohol is the ANZG Water Quality Guideline – Freshwater Trigger Value for alcohol ethoxylates.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Ethoxylated Branched C13 Alcohol (78330-21-9)	[a]	-	-	11.95

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Ethoxylated Branched C13 Alcohol (78330-21-9)	[a]	-	-	10.5

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x-y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerisation is indicated by the subscript (n) which indicates the average number of ethylene oxide units. Ethoxylated branched C13 alcohol has an average number of 1 to 7 moles of EO units.

Ethoxylated branched C13 alcohol is a substance of unknown or variable composition, complex reaction products or biological materials (UVCB). A representative molecular structure of an AE is presented in **Figure 1**.

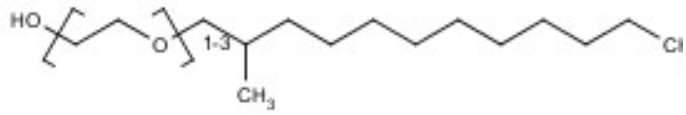

Figure 1 Molecular Structure of Ethoxylated branched C13 alcohol [2]

Ethoxylated branched C13 alcohol is readily biodegradable, is not likely to sorb to sediments or soil, and has low potential to bioaccumulate or bioconcentrate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for ethoxylated branched C13 alcohol is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the alcohol is not a PBT substance.

Human Health Hazards

The acute toxicity of ethoxylated branched C13 alcohol is low to moderate by the oral route and low via the dermal and inhalation routes of exposure. Neat ethoxylated branched C13 alcohol is expected to be irritating to the eyes of rabbits. However, the skin irritation rabbit studies have shown mixed results, and human patch studies on these AEs do not support a skin irritant classification. It is not a skin sensitiser. Repeated dose toxicity studies on AEs similar to ethoxylated branched C13 alcohol in rats do not indicate any target organ effects. These AEs are not genotoxic or carcinogenic and have a low potential for reproductive and developmental toxicity.

Based on a review of a two-year dietary study in rats, TRVs were derived for ethoxylated branched C13 alcohol. The drinking water guideline value derived for the substance using the non-carcinogenic oral RfD is 1.8 mg/L (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Ethoxylated branched C13 alcohol may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to ethoxylated branched C13 alcohol in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in recovered drilling and completion fluids would be diluted by at least 90% in the water feed pond due to the aggregation with produced water. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, ethoxylated branched C13 alcohol is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach,

[2] Source https://echa.europa.eu/brief-profile/-/briefprofile/100.105.729

other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

There are no aquatic toxicity studies for ethoxylated branched C13 alcohol. The aquatic toxicity of alcohols similar to ethoxylated branched C13 alcohol has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. AEs have moderate chronic toxicity to aquatic life.

Ethoxylated branched C13 alcohol is readily biodegradable, is not likely to sorb to sediments or soil, and has low potential to bioaccumulate or bioconcentrate. Therefore, while read-across AEs have been determined to be acutely toxic to aquatic organisms, if released to surface water, adverse effects would be localised due to its short half-life.

PNECs for ethoxylated branched C13 alcohol are provided in **Tables 3 – 5**. Ethoxylated branched C13 alcohol is an alcohol ethoxylate (AE). ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 0.14 mg/L for AE. This value was derived using data normalised to an alkyl chain length of C13.3 and EO of 8.2 using the statistical distribution method with 95% protection.

There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream

agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of ethoxylated branched C13 alcohol in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of ethoxylated branched C13 alcohol in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as ethoxylated branched C13 alcohol, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

ALCOHOLS, C11-14 -ISO, C13 RICH ETHOXYLATED

This dossier on alcohols, C11-14-iso, C13-rich ethoxylated (hereafter referred to as ethoxylated branched C13 alcohol) presents the most critical studies pertinent to the risk assessment of this substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products: Alcohol Ethoxylates (HERA, 2009), and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ethoxylated branched C13 alcohol was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Ethoxylated branched C13 alcohol was assessed as a tier 2 chemical for acute toxicity to fish. Ethoxylated branched C13 alcohol was assessed as a tier 3 chemical for acute toxicity to invertebrates and algae. Ethoxylated branched C13 alcohol was assessed as a tier 2 for chronic toxicity chemical to algae, invertebrates, and fish. Based on its potential for rapid degradation in the environment, it is not expected to pose a substantial toxic concern to environmental receptors. Therefore, this substance is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x\text{-}y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide (EO) polymerisation is indicated by the subscript (n) which indicates the average number of EO units. Ethoxylated branched C13 alcohol (CAS No. 78330-21-9) has an average number of 1 to 7 moles of EO units.

Ethoxylated branched C13 alcohol is readily biodegradable, is not likely to sorb to sediments or soil, and has low potential to bioaccumulate or bioconcentrate. The aquatic toxicity of alcohols similar to ethoxylated branched C13 alcohol has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. AEs have moderate chronic toxicity to aquatic life.

The acute toxicity of ethoxylated branched C13 alcohol is low to moderate by the oral route and low via the dermal and inhalation routes of exposure. Neat ethoxylated branched C13 alcohol is expected to be irritating to the eyes of rabbits. However, the skin irritation rabbit studies on ethoxylated branched C13 alcohol have shown mixed results, and human patch studies on these AEs do not support a skin irritant classification. It is not a skin sensitiser. Repeated dose toxicity studies on AEs similar to ethoxylated branched C13 alcohol in rats do not indicate any target organ effects. These AEs are not genotoxic or carcinogenic and have a low potential for reproductive and developmental toxicity.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Alcohols, C11-14 -iso, C13-rich ethoxylated

CAS RN:78330-21-9

Molecular formula: $–(CH_2)_{11-14}–(OCH_2CH_2)_n–OH$ (where n is the average number of EO units)

Molecular weight: Unspecified (Substance is a UVCB)

Synonyms: Ethoxylated C11-14-iso, C13 rich alcohol; ethoxylated branched C11-14, C13-rich alcohols; alpha-Alkyl-omega-hydroxypoly(oxypropylene) and/or poly(oxyethylene) polymers where the alkyl chain contains a minimum of six carbons, minimum number average molecular weight (in amu) 1,100

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Ethoxylated Branched C13 Alcohol*

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear liquid with rancy odour	2	ECHA
Melting Point	-11.6 °C @ 101.3 kPa	1	ECHA-
Boiling Point	>290°C @ 101.3 kPa	1	ECHA
Density	907 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	0.007 Pa @ 20°C	2	ECHA
Partition coefficient (log K_{ow})	4.73** (calculated) @25 °C	2	ECHA
Water Solubility	0.056 g/L @ 20°C	1	ECHA
Dissociation Constant (pKa)	Not applicable	-	ECHA
Viscosity	38.2 mm^2/s (kinematic) @ 20 °C	1	ECHA

*Information provided for read-across substance isotridecanol, ethoxylated (CAS No. 69011-36-5).
**Derived in a weight-of-evidence approach from various calculated log Pow values (average of values 4.55 and 4.90).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ethoxylated branched C13 alcohol.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Ethoxylated branched C13 alcohol is readily biodegradable. They are slightly soluble and have high adsorption potential to soil and sediment. However, they have a low potential to bioaccumulate.

B. Biodegradation

AE homologues with linear hydrocarbon chain lengths from C8 to C15 and mean values ranging from 3-20 EO units are readily biodegradable (HERA, 2009). Alcohols, C12-C14, ethoxylated (7-8) degraded to 100% in 28 days in a die away screening test (HERA, 2009) [Kl. Score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for ethoxylated branched C13 alcohol.

Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K_{oc} values for ethoxylated branched C13 alcohol are: 5,649 L/kg (MCI) and 20, 860 L/kg (K_{ow}). These values are within the range reported in HERA (2009) for alcohols, C11-C14, ethoxylated (7-8). However, as described in ECHA, one should keep in mind that surfactancy (the fact that surfactants tend to stay in the boundary layer between the phases) and dissociation is not considered in the EPISUITE™ estimations. Therefore, calculated K_{oc} values should be used with caution.

If released to soil, these K_{oc} values indicate a high potential for both adsorption and low potential for mobility. If released to water, based on these K_{oc} values and slight solubility, this substance is expected to strongly adsorb to suspended solids or sediment.

D. Bioaccumulation

There are no bioaccumulation studies on this substance.

The potential for bioaccumulation of AEs is considered low due to the biotransformation and excretion of the substance. The various studies present considerable evidence that AEs are rapidly eliminated and metabolised (ECHA).

The BCF values for AEs in fathead minnows have been reported to range from <5 to 387.5 (Toll et al., 2000). The uptake rates varied from 330 to 1660 (L x kg/day) and elimination rates varied from 3.3 to 59 per day (Toll et al., 2000). The high concentrations in fish are thought to be prevented by an efficient biotransformation of the AEs, leading to a high elimination rate. Thus, it can be stated that bioaccumulation of AEs is regarded to be negligible as the surfactants will be rapidly metabolised (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Overall, AEs are not expected to be systemically toxic. The available datasets for AEs ranging from C6–C18 and EO3–EO12 are considered representative of the AE category and were used to assess alcohols, C11-14-iso-, C13-rich, ethoxylated.

The acute toxicity of similar AEs is low to moderate by the oral route and low via the dermal and inhalation routes of exposure. Neat ethoxylated branched C13 alcohol is expected to be irritating to the eyes of rabbits. However, the skin irritation rabbit studies on ethoxylated branched C13 alcohol have shown mixed results, and human patch studies on these AEs do not support a skin irritant classification. It is not a skin sensitiser. Repeated dose toxicity studies on AEs similar to ethoxylated branched C13 alcohol in rats do not indicate any target organ effects. These AEs are not genotoxic or carcinogenic and have a low potential for reproductive and developmental toxicity.

B. Acute Toxicity

No acute toxicity studies are available on ethoxylated branched C13 alcohol.

Oral

The oral LD_{50} in rats for $C_{12\text{-}15}EO_3$ is >5,000 mg/kg (ECHA) [Kl. score = 2]. The oral LD_{50} in rats for $C_{12\text{-}15}EO_7$ is 1,700 mg/kg (HERA, 2009) [Kl. score = 2]. The oral LD_{50} value in rats for $C_{12\text{-}13}EO_{6.5}$ is 2,100 mg/kg (HERA, 2009) [Kl. score = 2]. The oral LD_{50} value in rats for $C_{12\text{-}15}EO_{11}$ is >2,000 mg/kg in males and between 1,000 and 2,000 mg/kg in females (HERA, 2009) [Kl. score = 2]. The relative number of EO units, but not the carbon chain length, appears to influence acute oral toxicity (HERA, 2009).

Dermal

Acute dermal LD_{50} values of 2,000 mg/kg were determined for $C_{12\text{-}14}EO_3$ and $C_{12\text{-}14}EO_6$ in two separate studies compliant with GLP and following OECD 402 guidelines (HERA, 2009) [Kl. score = 2]. The acute dermal LD_{50} of $C_{12\text{-}15}EO_7$ is >2000 mg/kg (HERA, 2009) [Kl. score = 2]. In rats, the dermal LD_{50} values ranged from >800 mg/kg bw ($C_{13\text{-}15}EO_{10}$, $C_{13\text{-}15}$ EO $_{11}$) to >5000 mg/kg bw (NICNAS, 2019) There is no apparent relationship between dermal toxicity and chemical structure with regard to alkyl chain length and the degree of ethoxylation for AEs (HERA, 2009; Talmage, 1994).

Inhalation

Based on the available data, the AEs in this group are expected to have low acute inhalation toxicity (NICNAS, 2019).

C. Irritation

Respiratory

Inhalation of droplets and/or particles (aerodynamic diameters <10 µm) released from the aerosolised products of these surfactant chemicals may cause respiratory irritation and consequent damage to the lung due to prolonged or repeated exposure (NICNAS, 2019).

Skin

In several OECD TG 404 (Acute Dermal Irritation/Corrosion) compliant tests, AEs of varying chain lengths were undiluted to intact rabbit skin for 4 hours under fully occluded conditions. The chemicals ranged from slightly irritating (C_{11} EO_9, $C_{12\text{-}14}EO_{15}$, $C_{13}EO_{20}$), moderately irritating ($C_{12\text{-}14}$ EO_{10}, $C_{13}EO_6$, $C_{13}EO_{5\text{-}6.5}$), to extremely irritating ($C_{12\text{-}14}EO_6$, $C_{12\text{-}14}EO_3$, $C_{13}EO_3$). The skin reaction from slightly irritating chemicals reversed by 6 days after exposure, and those from moderately to severely irritating chemicals persisted up to 14 days of the observation period. The data suggests a possible trend between irritation and degree of ethoxylation, i.e. AEs with lower EO units are likely more irritating than those with higher number of EO units (NICNAS, 2019).

After 24-hour occlusive application, the following AEs (undiluted) were moderately to severely irritating. For the same C12-13 alkyl length, AEs with EO3 were severely irritating while those with EO7 were mildly to severely irritating. Dilutions of these AEs were slightly to moderately irritating at 10% slightly irritating at 1% and minimally to non-irritating at 0.1% (NICNAS, 2019).

In a 24-hour human patch test, there was some short-lived redness in some individuals from the application of $C_{12\text{-}14}EO_3$, but there was no scaling or edema in any subjects (HERA, 2009) [Kl. Score = 2].

In a standard 4-hour human patch test, the irritation potential of $C_{12\text{-}15}EO_5$ and $C_{12\text{-}15}EO_5$ were compared to 20% sodium dodecyl sulfate (which is classified a skin irritant under GHS). The results showed that neither AE should be classified as a skin irritant (Basketter et al., 2004) [Kl. Score = 2]. Nonetheless, the substance is classified by ECHA as an irritant.

Undiluted AEs (covering the range of C11-C18 and EO3-E020) were reported to cause mild skin irritation in several standard human occlusive patch tests (4-24 hours). In some cases, mild erythema was observed and cleared within 72 hours (NICNAS, 2019).

In a human sensitisation test, the chemical C12-13 EO6.5 showed an increased cumulative irritation response compared to AEs with a higher degree of ethoxylation, e.g. $C_{12\text{-}15}$ EO_{12} (NICNAS,2019).

Eye

Most AEs tested as the undiluted neat test material are moderately to severely irritating to the eyes of rabbits, with an eye irritation index (EII) ranging from >25 to 50 (HERA, 2009). The severity of

irritation was considered concentration-dependent and appears to not correlate with ethoxylation or alkyl chain length of the AEs (NICNAS, 2019).

The AEs $C_{12\text{-}14}EO_3$, $C_{12\text{-}14}EO_6$, $C_{13}EO_6$, and $C_{12\text{-}14}EO_{10}$ were found to be moderately to severely irritating to the eyes of rabbits (HERA, 2009). Other AEs (i.e., $C_{12\text{-}13}$ EO_2) EII scores of 0.5 to 15 (mildly irritating) Thus, there is no clear pattern between the eye irritant responses versus the alkyl or EO chain lengths (NICNAS, 2009).

D. Sensitisation

No sensitisation studies are available on ethoxylated branched C13 alcohol.

In a guinea pig maximisation tests, $C_{12\text{-}15}EO_3$ and $C_{12\text{-}15}EO_7EO$ were not considered skin sensitisers (HERA, 2009) [Kl. scores = 2].

A number of AEs of varying chain lengths, e.g. $C_{12\text{-}C18}$ and EO2-EO23 [including $C_{12\text{-}13}$ $EO_{6.5}$ (CAS No. 66455-14-9) and $C_{12\text{-}15}$ $EO_{7\text{-}12}$ (CAS No. 68131-39-5)] all tested negative in human repeated insult patch tests (HRIPTs). Induction concentrations were mostly between 1-25% (NICNAS, 2019)

E. Repeated Dose Toxicity

Oral

No repeated dose toxicity studies are available on ethoxylated branched C13 alcohol. Data for similar AEs are presented below.

Rats were given in their diet 0%, 0.0313%, 0.0625%, 0.125, 0.25, 0.5 or 1.0% $C_{12\text{-}15}EO_7$ for 90 days. The animals in the ≥0.25% groups showed significantly reduced body weight gain, which was associated with marked decreases in food and water consumption. Relative liver weights were significantly increased in the ≥0.5% male rats and ≥0.25% females. Histopathologic examination showed hepatocytic enlargement in the ≥0.125% groups, suggesting increased liver metabolism on the basis of increased alkaline phosphatase activity at the higher dose levels. The NOAEL was established at 0.125% in the diet or 102 mg/kg-day (HERA, 2009) [Kl. score = 2].

Rats were fed $C_{12\text{-}14}EO_7$ in the diet at concentrations of 0%, 0.0313%, 0.0625%, 0.125%, 0.25%, 0.5% and 1.0% for 90 days. The animals in the ≥0.25% groups showed significantly reduced body weight gain, which was associated with marked decreases in food and water consumption. Relative liver weights were significantly increased in the ≥0.5% male rats and ≥0.25% females. Histopathologic examination showed hepatocytic enlargement in the ≥0.125% groups, suggesting increased liver metabolism on the basis of increased alkaline phosphatase activity at the higher dose levels. The NOAEL was established at 0.125% in the diet or 110 mg/kg-day (HERA, 2009) [Kl. score = 2].

Rats were given in their diet 0, 0.1, 0.5 or 1% $C_{12\text{-}13}EO_{6.5}$ or $C_{14\text{-}15}EO_7$ for two years. Body weight gain was reduced in the 1% males and ≥0.5% females, which was likely due to the reduced food consumption in these animals. At study termination, organ to body weight ratios were increased in the ≥0.5% females (liver, kidney and brain), 1% females (heart), and 1% males (liver). A dose-related focal myocarditis was observed in males. While focal myocarditis is commonly observed in non-treated aging rats, the incidence in the treated animals were higher than in the controls. The NOAEL was established at 0.1% or 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Inhalation

No studies are available.

Dermal

In an 18-month study, C_{12-13} EO $_{6.5}$ was applied to the back of Swiss mice 3 days/week. There were no treatment-related systemic lesions at up to 270 mg/kg bw/day. No further study information was available (NICNAS, 2019).

F. Genotoxicity

Based on the data available, the chemicals in this group are not considered mutagenic or genotoxic. A broad spectrum of AEs (covering the range of C7–C22 and EO2–EO20) tested negative in multiple in vitro and in vivo tests (OECD and GLP compliant) for gene mutation and clastogenicity (NICNAS, 2019).

In Vitro Studies

In vitro, negative results were reported in bacterial reverse mutation tests in *Salmonella typhimurium* (TA98, TA100, TA102, TA104, TA1535, TA1537 and TA1538) and *Escherichia coli* (strains WP2 and WP2 uvrA pKM101), with or without metabolic activation. Negative results were also reported in chromosomal aberration tests (Chinese hamster lung V79, Chinese hamster ovary, and rat liver cells) and gene mutation tests (mouse lymphoma cells) (NICNAS, 2019).

In Vivo Studies

In two separate studies, CD-1 mice were given an intraperitoneal dose of 0, 50, or 100 mg/kg $C_{12-15}EO_3$ or $C_{12-14}EO_9$. There were no increases in the frequency of micronuclei in the bone marrow cells (Talmage, 1994) [Kl. score = 2].

In vivo, AEs (C12-C15 and EO3-E09) did not induce chromosomal damage in Chinese hamster or Tunstall Wistar rat bone marrow cells after acute oral doses between 250 and 3400 mg/kg bw (NICNAS,2019).

G. Carcinogenicity

No studies are available on ethoxylated branched C13 alcohol. Therefore, data for similar substances are presented below.

Male and female Sprague-Dawley rats were given in their diet $C_{12-13}EO_{6.5}$ in the diet at doses up to 1% (500 mg/kg-day). Reduced food consumption was noted at the higher dose levels (*i.e.*, 0.5 and 1% for females and 1% for males), resulting in a lower body weight gain compared to the control group. No treatment-related histopathology was found and no increase in tumour incidence was observed (HERA, 2009) [Kl. score = 2].

AE C_{12-13} EO $_{6.5}$ (CAS No. 66455-14-9) was administered at up 1% in diet to rats 1-2 years. No treatment-related histopathological effects or increased tumour incidence were observed (NICNAS, 2019).

There were no treatment-related lesions in mice, following 18-month dermal application of C_{12-13}

$EO_{6.5}$ (NICNAS, 2019).

H. Reproductive Toxicity

No studies are available on ethoxylated branched C13 alcohol.

CD rats were given in their diet 0, 0.05, 0.1 or 0.5% (approximately 0, 25, 50 or 250 mg/kg-day) $C_{12}EO_6$ in a two-generation reproductive toxicity study. There were no treatment related effects in the parents or pups on general behaviour, appearance or survival. At 0.5%, there was reduced weight gain in both the parental animals and the pups compared to the controls. Fertility was unaffected by treatment. The NOAEL for reproductive toxicity is 0.5% in the diet, which corresponds to 250 mg/kg-day (HERA, 2009) [Kl. score = 2].

I. Developmental Toxicity

No studies are available on ethoxylated branched C13 alcohol.

In a two-generation reproductive toxicity study, Charles River rats were given in their diet 0, 0.05, 0.1 or 0.5% (about 0, 25, 50 or 250 mg/kg-day) $C_{12}EO_6$. General behaviour, appearance and survival were unaffected by treatment. At the 0.5% dose level, adults and pups gained less weight than the control rats. In the 0.5% dose group, there was a statistical increase in embryo lethality and soft tissue anomalies and at the 0.1% there was a statistical decrease in mean fetal liver weight. Neither of these effects was considered to be treatment-related by the authors as they showed no dose response characteristics. The NOAEL for maternal toxicity is 50 mg/kg-day. The NOAEL for developmental and teratogenicity is 0.1% in the diet or 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Pregnant rabbits were given by oral gavage 0, 50, 100 or 200 mg/kg $C_{12}AE$ from gestational days 2 to 16. Nine control rabbits and 31 treated rabbits died during the study. Surviving rabbits at the 200 mg/kg dose group generally showed slight losses of body weight. At 100 and 200 mg/kg, ataxia and a slight decrease in body weight was observed in the pregnant animals. In seven treated and two control rabbits, early deliveries were recorded. There were no treatment-related effects on corpora lutea, implantations, number of live fetuses and spontaneous abortions. The NOAEL for maternal toxicity is 50 mg/kg-day; the NOAEL for developmental toxicity is 200 mg/kg-day (HERA, 2009) [Kl. score = 2].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for ethoxylated branched C13 alcohol follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

<u>Non-Cancer</u>

A two-year dietary study in rats has been conducted on AEs $C_{12\text{-}13}EO_{6.5}$ (HERA, 2009). The NOAEL from this study is 50 mg/kg-day based on increased organ weights. This NOAEL will be used to derive an oral reference dose and drinking water guidance value for ethoxylated branched C13 alcohol.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:

UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 50/(10 x 10 x 1 x 1 x 1) = 50/100 = 0.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:

Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.5 x 70 x 0.1)/2 = 1.8 mg/L

Cancer

Several AEs similar to ethoxylated branched C13 alcohol were not carcinogenic to rats in a two-year dietary study. Thus, a cancer reference value was not derived.

K. HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

Ethoxylated branched C13 alcohol does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

There are no aquatic toxicity studies for ethoxylated branched C13 alcohol. The aquatic toxicity of other AEs has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. AEs have moderate chronic toxicity to aquatic life.

B. Aquatic Toxicity

Acute Studies

There are no acute aquatic toxicity studies for ethoxylated branched C13 alcohol. The aquatic toxicity of other AEs has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. Table 3 lists the results of acute aquatic toxicity studies on read across substance alcohols, C12-C14, ethoxylated (2 EO) [CAS No. 68439-50-9].

Table 3 Acute Aquatic Toxicity Studies on Ethoxylated Branched C13 Alcohol[a,b,c]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio Rio	96-hr LC_{50}	1.2[a]	2	ECHA
Danio Rio	96-hr LC_{50}	2[a]	2	ECHA
Daphnia magna	48-hr EC_{50}	0.53[a]	2	ECHA
Daphnia magna	48-hr EC_{50}	2.84[a,b]	2	ECHA
Daphnia magna	48-hr EC_{50}	1.2[c]	1	ECHA
Daphnia magna	48-hr EC_{50}	>2[a]	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	>2[c]	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	0.41[a]	2	ECHA
Desmodesmus subspicatus (green algae)	72-hr EC_{50}	0.778[a]	2	ECHA
Desmodesmus subspicatus (green algae)	72-hr EC_{50}	0.87[c]	1	ECHA
Desmodesmus subspicatus (green algae)	72-hr EC_{50}	1.3[c]	1	ECHA

a: Read across to alcohols, C12-C14, ethoxylated (EO 2) CAS No. 68439-50-9
b: alcohols, C12-C14, ethoxylated (EO 1) CAS No. 68439-50-9 as WAF (water accommodated fraction)
c: alcohols, C12-C14, ethoxylated (EO 4 or EO 6) CAS No. 68439-50-9

A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. As concluded in HERA (2009), the Danish EPA (2001) found that the acute toxicity of AE to invertebrates varies, with EC_{50} values from 0.1 mg/l to more than 100 mg/l for linear AE and from 0.5 mg/l to 50 mg/l for branched AE. The toxicity is species specific and may vary between 0.29 mg/l and 270 mg/l for the same linear AE (Lewis and Suprenant 1983, quoted in Danish EPA 2001). The most commonly used invertebrates for testing are Daphnia magna and Daphnia pulex, and they are also among the most sensitive invertebrates to AE. The Danish EPA (2001) found that some AE are very toxic to invertebrates, i.e., linear AE of C12-15 EO1-8 and branched AE with a low degree of branching, i.e. < 10-25%. They concluded that branching of the alkyl chain reduces the toxicity of AE to invertebrates, as also observed for algae (Danish EPA 2001). However, the data used to reach this conclusion is from specially synthesised AE which have been shown to have a significantly higher

toxicity than the AE made from a technical alcohol which are used commercially (Kaluza and Taeger, 1996).

Chronic Studies

In developing a water quality guideline for AEs (ANZG, 2018), the toxicity data was normalised for a specific alkyl chain length or a specific number of EO groups. The NOECs listed below were normalised to an alkyl chain length of C13.3 and EO of 8.2. There were chronic data for 13 species that belonged to 7 taxonomic groups (fish, crustacea, blue alga, diatoms, green alga, protozoa, and worms).

Freshwater fish: 2 species, 720 to 1,500 µg/L.

Freshwater crustaceans: 2 species, 590 to 860 µg/L.

Freshwater rotifers: 1 species, *Brachionus calyciflorus*, 1,300 µg/L.

Freshwater algae, diatoms and blue-green algae: 6 species, 200 to 8,700 µg/L.

Freshwater mesocosms: 4 NOEC data for multiple species tests were 80, 80, 320 and 330 µg/L, although replication was insufficient to meet OECD (1992) requirements. Normalised data were 380, 380, 320 and 1,520 µg/L.

C. Terrestrial Toxicity

No studies are available. The substance is readily biodegradable. Therefore, soil is not expected to be a compartment of concern. Thus, the risk to terrestrial organisms is regarded to be negligible (ECHA).

D. Calculation of PNEC

The PNEC calculations for ethoxylated branched C13 alcohol follow the methodology discussed in DEWHA (2009).

PNEC water

The ANZG water quality guideline (2018) in freshwater is: “A high reliability trigger value of 140 µg/L (0.14 mg/L) was derived for AE (normalised data) using the statistical distribution method with 95% protection.”

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Nonetheless, a $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 11.95 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 109/1280 \times 1000 \times 0.140$
$= 11.95$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = 0.14 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 2.26E02)/1000 \times 2400]$
$= 109\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]
$Kp_{sed} = K_{oc} \times f_{oc}$
$= 5649 \times 0.04$
$= 226$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for ethoxylated branched C13 alcohol based on the molecular connectivity index (MCI) is 5649 L/kg (USEPA, 2018). The MCI method is preferred to the K_{ow} method due to the surfactant properties of the substance.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 10.5 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (113/1500) \times 1000 \times 0.14$
$= 10.54$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 kg/m^3 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 5649 \times 0.02$
$= 113\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for ethoxylated branched C13 alcohol based on the molecular connectivity index (MCI) is 5649 L/kg (USEPA, 2018).
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Ethoxylated branched C13 alcoholis readily biodegradable and thus does not meet the screening criteria for persistence.

The bioconcentration factors (BCF) in fish for ethoxylated alcohols (which includes ethoxylated branched C13 alcohol) have been reported to range from <5 to 387.5. Thus, ethoxylated branched C13 alcoholdoes not meet the screening criteria for bioaccumulation.

The chronic NOEC values for AEs are > 0.1 mg/L. Thus, ethoxylated branched C13 alcohol does not meet the criteria for toxicity.

Thus, ethoxylated branched C13 alcohol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ethoxylated branched C13 alcohol.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Alcohols, C11-14-iso, C13-rich ethoxylated	78330-21-9	Not a PBT	No	No	No	No	No	No	2 (fish) and 3 (inverts and algae)	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). Acute aquatic toxicity for invertebrates and algae range between 0.41 and 2.84 mg/L with variability likely due to varying test conditions and differences in chemical structure. Average results are greater than 1.

3 – Tier 2 – Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
AE	alcohol ethoxylates
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Environment Guidelines
BCF	bioconcentration factor
bw	body weight
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EO	ethylene oxide

EU	European Union
g/L	grams per litre
HERA	Human and Environmental Risk Assessment
HRIPT	Human Repeat Insult Patch Test
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
K_{oc}	octanol-water partition coefficient
K_{ow}	octanol-water partition coefficient
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/kg bw/day	milligrams per kilogram body weight per day
mg/L	milligrams per litre
mPa s	millipascal second
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
µg/L	micrograms per litre
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
Ethoxylated alcohol	78330-21-9	1.65E+00	1.50E+01	1.65E-01	4.13E-02	1.65E-03	4.13E-04	3.30E-05	8.25E-06	1.40E-01

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Ethoxylated C12-C16 Alcohol

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk (an incomplete pathway precludes an exposure occurring and an associated potential risk). In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Ethoxylated C12-C16 alcohol is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Ethoxylated C12-C16 Alcohol	68551-12-2	Crosslinker	0.00015%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. Several alcohol ethoxylates similar to ethoxylated C12-C16 alcohol were not carcinogenic to rats in a two-year dietary study. Thus, a cancer reference value was not derived. As a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Ethoxylated C12-C16 Alcohol (CAS No. 68551-12-2)	2-yr Dietary Study	Increased organ weight	50	100	0.5	1.8

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Ethoxylated C12-C16 Alcohol (CAS No. 68551-12-2)	-	-	-	0.14[a]

$PNEC_{water}$ for ethoxylated C12-C16 alcohol is the ANZG Water Quality Guideline – Freshwater Trigger Value for alcohol ethoxylates.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Ethoxylated C12-C16 Alcohol (CAS No. 68551-12-2)	[a]	-	-	0.0875

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Ethoxylated C12-C16 Alcohol (CAS No. 68551-12-2)	[a]	-	-	7.32

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x-y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerisation is indicated by the subscript (n) which indicates the average number of ethylene oxide units. Ethoxylated C12-C16 alcohol has an average number of 1 to 6 moles of ethylene oxide units.

Ethoxylated C12-C16 alcohol is a substance of unknown or variable composition, complex reaction products or biological materials (UVCB). A representative molecular structure of an AE is presented in **Figure 1**.

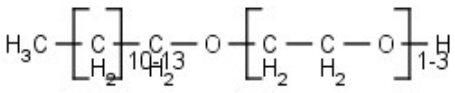

Figure 1 Molecular Structure of Ethoxylated C12-C16 alcohol [2]

Ethoxylated C12-C16 alcohol is readily biodegradable. It has a low potential for bioaccumulation and is unlikely to adsorb to soil or sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for ethoxylated C12-C16 alcohol is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

Ethoxylated C12-C16 alcohol exhibits low acute toxicity by the oral and dermal routes. The skin irritation rabbit studies on alcohols, C12-16, ethoxylated have shown mixed results, but human patch studies on these alcohol ethoxylates do not support a skin irritant classification. Alcohols, C12-16, ethoxylated is expected to be irritating to the eyes of rabbits. Alcohols, C12-16, ethoxylated is not a skin sensitizer. Repeated dose toxicity studies on alcohol ethoxylates similar to alcohols, C12-16, ethoxylated in rats do not indicate any target organ effects. These alcohol ethoxylates are not genotoxic, carcinogenic, and have a low potential for reproductive and developmental toxicity.

In a two-year dietary study conducted in rats alcohol ethoxylates $C_{12-13}AE_{6.5}$ and $C_{14-15}AE_{7}$ organ to body weight ratios were increased females. A no observed adverse effect level (NOAEL) of 50 mg/kg bw/day was established. This NOAEL was used for determining the oral RfD and the drinking water guideline value (1.8 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Alcohols, C12-16, ethoxylated may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to alcohols, C12-16, ethoxylated in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, alcohols, C12-16, ethoxylated is readily biodegradable and does not persist in the environment.

[2] Source https://echa.europa.eu/brief-profile/-/briefprofile/100.105.687

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

There are no aquatic toxicity studies for ethoxylated C12-C16 alcohol. The aquatic toxicity of other AEs has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. AEs have moderate chronic toxicity to aquatic life.

Ethoxylated C12-C16 alcohol is readily biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation. Therefore, while read-across AEs have been determined to be acutely toxic , if released to surface water, adverse effects would be localised due to its short half-life.

PNECs for ethoxylated C12-C16 alcohol are provided in **Tables 3-5**. Ethoxylated C12-C16 alcohol is an alcohol ethoxylate (AE). ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 0.14 mg/L for AE. This value was derived using data normalised to an alkyl chain length of C13.3 and EO of 8.2 using the statistical distribution method with 95% protection. Considering the land uses adjacent to the Dawson River include light to moderate grazing, and there is some development upstream of the Horseshoe Lakes, adoption of the 95% species protection criteria is considered appropriate (AECOM, 2019).

There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of ethoxylated C12-C16 alcohol in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, first, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The concentration of ethoxylated C12-C16 alcohol within the stimulation fluids will decrease in response to biodegradation and photolytic degradation of constituents over time. Chemical-specific biodegradation information presented in the dossier was used for the assessment.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Santos, 2013. Dawson River Release Scheme – Environmental Authority Amendment Application – Supporting Information. May 2013.

Attachment 1 Risk Assessment Dossier

ETHYOXYLATED C12-C16 ALCOHOL

This dossier on ethoxylated C12-C16 alcohol presents the most critical studies pertinent to the risk assessment of this substance in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products: Alcohol Ethoxylates (HERA, 2009), and from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ethoxylated C12-C16 Alcohol was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Ethoxylated C12-C16 Alcohol was assessed as a tier 2 chemical for acute toxicity of fish, a tier 3 chemical for acute toxicity of invertebrates and algae, and a tier 2 chemical for chronic toxicity of fish, invertebrates and algae. Based on its potential for rapid degradation in the environment, it is not expected to pose a substantial toxic concern to environmental receptors. Therefore, this substance is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x\text{-}y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide (EO) polymerisation is indicated by the subscript (n) which indicates the average number of EO units. Ethoxylated C12-C16 alcohol (CAS No. 68551-12-2) has an average number of 1 to 6 moles of ethylene oxide units.

Ethoxylated C12-C16 alcohol is readily biodegradable, is not likely to sorb to sediments or soil, and has low potential to bioaccumulate or bioconcentrate. There are no aquatic toxicity studies for ethoxylated C12-C16 alcohol. The aquatic toxicity of other AEs has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. AEs have moderate chronic toxicity to aquatic life.

The acute toxicity of alcohols, C12-16, ethoxylated is low by the oral and dermal routes. The skin irritation rabbit studies on alcohols, C12-16, ethoxylated have shown mixed results, but human patch studies on these alcohol ethoxylates do not support a skin irritant classification. Alcohols, C12-16, ethoxylated is expected to be irritating to the eyes of rabbits. Alcohols, C12-16, ethoxylated is not a skin sensitizer. Repeated dose toxicity studies on alcohol ethoxylates similar to alcohols, C12-16, ethoxylated in rats do not indicate any target organ effects. These alcohol ethoxylates are not genotoxic, carcinogenic, and have a low potential for reproductive and developmental toxicity.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Alcohols, C12-16, ethoxylated

CAS RN: 68551-12-2

Molecular formula: $H–(CH_2)_{12–16}–(OCH_2CH_2)_n–OH$ (where n is the average number of EO units)

Molecular weight: Unspecified (Substance is a UVCB)

Synonyms: Ethoxylated C12-16 alcohols; polyethylene glycol, dodecyl, tetradecyl, hexadecyl ether

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Ethoxylated C12-16 Alcohols[1]

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear liquid with a rancid odour*	2	ECHA
Melting Point	7.22°C	2	ECHA
Boiling Point	ca. 287°C	1	ECHA
Density	0.926 g/cm^3 @ 15.56°C	1	ECHA
Vapour Pressure	Negligible	-	ECHA
Partition coefficient (log K_{ow})	5.06* @ 25°C	2	ECHA
Water Solubility	7 – 63 mg/L @ 25°C	2	ECHA
Viscosity	28.1 mPA s (dynamic) @ 20°C	2	ECHA

1 – Based on alcohols, C12-C15, ethoxylated (1 to 2.5 EO) [CAS No. 68131-39-5]
*Based on alcohols, C12-14, ethoxylated (1 to 2.5 EO) [CAS No. 68439-50-9]

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ethoxylated C12-C16 alcohol.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No

Convention, Protocol or other international control	Listed Yes or No?
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Ethoxylated C12-C16 alcohol is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for absorption to soil and sediment.

B. Biodegradation

AE homologues with linear hydrocarbon chain lengths from C8 to C15 and mean values ranging from 3-20 EO units are readily biodegradable (HERA, 2009). If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

Alcohols, C12-C14, ethoxylated (7-8) degraded to 100% in 28 days in a die away screening test (HERA, 2009) [Kl. Score = 2].

Alcohols, C12-15, ethoxylated is readily biodegradable. In an OECD 301B test, degradation was 72% in 28 days, but failed the 10-day window (ECHA) [Kl. score = 1].

An alcohol, C12-15, ethoxylated (7 EO) degraded 80 to 88% in 28 days when tested using a shake-flask CO_2-evolution test method (ECHA) [Kl. score = 2].

C. Environmental Distribution

No experimental data are available for ethoxylated C12-C16 alcohol. Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K_{oc} values for ethoxylated C12-C16 alcohol are: 3,920 L/kg (MCI) and 13,530 L/kg (K_{ow}). Based on this K_{oc} value, if released to soil, the substance is expected to strongly adsorb to soil and have a low potential for mobility.

D. Bioaccumulation

The potential for bioaccumulation of AEs is considered low due to the biotransformation and excretion of the substance. The various studies present considerable evidence that AEs are rapidly eliminated and metabolised (ECHA).

The BCF values for AEs in fathead minnows have been reported to range from <5 to 387.5 (Toll et al., 2000). The uptake rates varied from 330 to 1660 (L x kg/day) and elimination rates varied from 3.3 to 59 per day (Toll et al., 2000). The high concentrations in fish are thought to be prevented by an efficient biotransformation of the AEs, leading to a high elimination rate.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of alcohols, C12-16, ethoxylated is low by the oral and dermal routes. The skin irritation rabbit studies on alcohols, C12-16, ethoxylated have shown mixed results, but human patch studies on these alcohol ethoxylates do not support a skin irritant classification. Alcohols, C12-16, ethoxylated is expected to be irritating to the eyes of rabbits. Alcohols, C12-16, ethoxylated is not a skin sensitizer. Repeated dose toxicity studies on alcohol ethoxylates similar to alcohols, C12-16, ethoxylated in rats do not indicate any target organ effects. These alcohol ethoxylates are not genotoxic, carcinogenic, and have a low potential for reproductive and developmental toxicity.

B. Acute Toxicity

No acute toxicity studies are available on alcohols, C12-16, ethoxylated.

The oral LD_{50} in rats for $C_{12\text{-}15}AE_3$ is >5,000 mg/kg (ECHA) [Kl. score = 2]. The oral LD_{50} in rats for $C_{12\text{-}15}AE_7$ is 1,700 mg/kg (HERA, 2009) [Kl. score = 2]. The oral LD_{50} value in rats for $C_{12\text{-}13}AE_{6.5}$ is 2,100 mg/kg (HERA, 2009) [Kl. score = 2]. The oral LD_{50} value in rats for $C_{12\text{-}15}AE_{11}$ is >2,000 mg/kg in males and between 1,000 and 2,000 mg/kg in females (HERA, 2009) [Kl. score = 2]. The oral LD_{50} values in rats for $C_{14\text{-}15}AE_{13}$ in two separate studies are 1,100 and 1,000 mg/kg (HERA, 2009) [Kl. score = 2]. The relative number of EO units, but not the carbon chain length, appears to influence acute oral toxicity (HERA, 2009).

Acute dermal LD_{50} values of >2,000 mg/kg were determined for $C_{12\text{-}14}AE_3$ and $C_{12\text{-}14}AE_6$ in two separate studies (HERA, 2009) [Kl. score = 2]. The acute dermal LD_{50} of $C_{12\text{-}15}AE_7$ is >2,000 mg/kg (HERA, 2009) [Kl. score = 2].

C. Irritation

Skin

Application of 0.5 mL isotridecanol, ethoxylated (3 EO) to the skin of rabbits for 4 hours under occlusive conditions was considered irritating (ECHA) [Kl. score = 2].

Application of 0.5 mL isotridecanol, ethoxylated (3 EO) to the skin of rabbits for 4 hours under semi-occlusive conditions was not considered irritating (ECHA) [Kl. score = 2].

In a 24-hour human patch test, there was some short-lived redness in some individuals from the application of $C_{12\text{-}14}AE_3$, but there was no scaling or edema in any subjects (HERA, 2009) [Kl. score = 2].

In a standard 4-hour human patch test, the irritation potential of $C_{12\text{-}15}AE_5$ and $C_{12\text{-}15}AE_5$ were compared to 20% sodium dodecyl sulfate (which is classified a skin irritant under GHS). The results showed that neither alcohol ethoxylate should be classified as a skin irritant (Basketter et al., 2004) [Kl. score = 2]. Nonetheless, the substance is classified by ECHA as an irritant.

Eye

Most alcohol ethoxylates tested as the undiluted neat test material are moderately to severely irritating to the eyes of rabbits, with an eye irritation index (EII) ranging from >25 to 50 (HERA, 2009).

The alcohol ethoxylates $C_{12-14}AE_3$, $C_{12-14}AE_6$, $C_{13}AE_6$, and $C_{12-14}AE_{10}$ were found to be moderately to severely irritating to the eyes of rabbits (HERA, 2009). In another study, $C_{12-15}AE_{11}$ was considered moderately to severely irritating to the eyes of rabbits (HERA, 2009).

Some alcohol ethoxylates were reported to be practically or minimally irritating to the eyes of rabbits with EII scores of 0.5 to 15. These alcohol ethoxylates include: $C_{12-15}AE_3$, $C_{14-15}AE_7$, $C_{12-14}AE_{15}$, $C_{14-15}AE_{18}$, and $C_{13}AE_{20}$ (HERA, 2009).

D. Sensitisation

No sensitisation studies are available on alcohols, C12-16, ethoxylated.

In a guinea pig maximization test, $C_{12-13}AE_{<2.5}$ (CAS No. 66455-14-9) was not considered a skin sensitiser (ECHA) [Kl. score = 2].

In a guinea pig maximization tests, $C_{12-15}AE_3$, $C_{12-15}AE_7$, and $C_{14-15}AE_7$ were not considered skin sensitisers (HERA, 2009) [Kl. scores = 2].

E. Repeated Dose Toxicity

Oral

No repeated dose toxicity studies are available on alcohols, C12-16, ethoxylated. Data for similar ethoxylates are presented below.

Rats were given in their diet 0%, 0.0313%, 0.0625%, 0.125, 0.25, 0.5 or 1.0% $C_{12-15}AE_7$ for 90 days. The animals in the ≥0.25% groups showed significantly reduced body weight gain, which was associated with marked decreases in food and water consumption. Relative liver weights were significantly increased in the ≥0.5% male rats and ≥0.25% females. Histopathologic examination showed hepatocytic enlargement in the ≥0.125% groups, suggesting increased liver metabolism on the basis of increased alkaline phosphatase activity at the higher dose levels. The NOAEL was established at 0.0625% in the diet or 102 mg/kg-day (HERA, 2009) [Kl. score = 2].

Rats were fed $C_{12-14}AE_7$ in the diet at concentrations of 0%, 0.0313%, 0.0625%, 0.125%, 0.25%, 0.5% and 1.0% for 90 days. The animals in the ≥0.25% groups showed significantly reduced body weight gain, which was associated with marked decreases in food and water consumption. Relative liver weights were significantly increased in the ≥0.5% male rats and ≥0.25% females. Histopathologic examination showed hepatocytic enlargement in the ≥0.125% groups, suggesting increased liver metabolism on the basis of increased alkaline phosphatase activity at the higher dose levels. The NOAEL was established at 0.0625% in the diet or 110 mg/kg-day (HERA, 2009) [Kl. score = 2].

Male and female Wistar rats given in their diet 0, 300, 1,000, 3,000, and 10,000 ppm $C_{14-15}AE_7$ for 90 days. There were no deaths during the study. Mean body weights and feed were lower in 10,000 ppm males and the 3,000 ppm females. Feed consumption was lower in the 10,000 ppm animals and the 3,000 ppm females. Relative liver weights were increased in the ≥3,000 ppm animals, and relative spleen weights were increased in the 10,000 ppm males. Clinical chemistry changes were noted in the 10,000 ppm group and consisted of significantly higher urea, chloride and potassium levels in males; significantly higher urea, chloride and cholesterol in females. Increased total leucocytes and lymphocytes were seen in the 10,000 ppm animals and in the 3,000 ppm males. The 10,000 ppm females showed lower numbers of neutrophils; mean cell volume and mean cell

hemoglobin were identified in one or both sexes fed in the ≥3,000 ppm dose groups. In the 1,000 ppm females, there were minor, but statistically significant changes in the liver and kidney weights and plasma urea concentration; these effects were considered to be of no toxicological significance. Histopathologic examination showed no treatment-related effects at any dose level. The NOAEL for this study is 1,000 ppm in the diet, which corresponded to 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Rats were given in their diet 0, 0.1, 0.5, or 1% $C_{14\text{-}15}AE_7$ for 90 days. Body weights, food intake, organ weights, and hematology and clinical chemistry parameters were similar across groups. The NOAEL for this study is 1% in the diet, which corresponded to 700 and 785 mg/kg-day for males and females, respectively (HERA, 2009) [Kl. score = 2].

Rats were given in their diet 0, 0.1, 0.5 or 1% $C_{12\text{-}13}AE_{6.5}$ or $C_{14\text{-}15}AE_7$ for two years. Body weight gain was reduced in the 1% males and ≥0.5% females, which was likely due to the reduced food consumption in these animals. At study termination, organ to body weight ratios were increased in the ≥0.5% females (liver, kidney and brain), 1% females (heart), and 1% males (liver). A dose-related focal myocarditis was observed in males. While focal myocarditis is commonly observed in non-treated aging rats, the incidence in the treated animals were higher than in the controls. The NOAEL was established at 0.1% or 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Male and female CR rats were given in their diet $C_{14\text{-}15}AE_7$ at 0.1, 0.5 and 1% for two years. A treatment-related body weight depression was observed in females at the two highest treatment levels and in males at the 1% dose level, probably due to the poor palatability of the diet. Relative liver, kidney, heart, and thyroid/parathyroid gland weights were increased in the 1% dietary group at study termination. Histopathological examination showed a dose-related increase in the incidence of focal myocarditis at the 12-month time point, but not at the end of the study at two years. The NOAEL for this study was considered to be 0.5% in the diet, which corresponded to 162 and 190 mg/kg-day for males and females, respectively (HERA, 2009) [Kl. score = 2].

Inhalation

No studies are available.

Dermal

No adequate studies are available.

F. Genotoxicity

In Vitro Studies

The genotoxicity studies conducted on alcohol ethoxylates are reviewed in HERA (2009). The results of few of the *in vitro* studies on similar alcohol ethoxylates to alcohols, C12-16, ethoxylated are presented below in Table 3.

Table 3: *In Vitro* Genotoxicity Studies on Selected Alcohol Ethoxylates

Test Substance	Test System	Results*		Klimisch Score	References
		-S9	+S9		
$C_{14\text{-}15}AE_7$	Bacterial reverse mutation (*S. typhimurium* strains)	-	-	2	HERA, 2009
$C_{14\text{-}15}AE_7$	Bacterial reverse mutation (*S. typhimurium* strains)	-	-	2	HERA, 2009
$C_{14}AE_{12}$	Chromosomal aberrations (CHO cells)	-	-	2	HERA, 2009

*+, positive; -, negative

In Vivo Studies

In two separate studies, CD-1 mice were given an intraperitoneal dose of 0, 50, or 100 mg/kg $C_{12\text{-}15}AE_3$ or $C_{12\text{-}14}AE_9$. There were no increases in the frequency of micronuclei in the bone marrow cells (Talmage, 1994) [Kl. score = 2].

Male and female Tunstall rats were given a single oral gavage dose of 0, 250, 500, or 1,000 mg/kg $C_{14\text{-}15}AE_7$. There were no increases in chromosomal aberrations in the bone marrow cells (HERA, 2009 [Kl. score = 2].

G. Carcinogenicity

No studies are available on alcohols, C12-16, ethoxylated. Therefore, data from similar substances are presented below.

Male and female Sprague-Dawley rats were given in their diet $C_{12\text{-}13}AE_{6.5}$ in the diet at doses up to 1% (500 mg/kg-day). Reduced food consumption was noted at the higher dose levels (*i.e.*, 0.5 and 1% for females and 1% for males), resulting in a lower body weight gain compared to the control group. No treatment-related histopathology was found and no increase in tumor incidence was observed (HERA, 2009) [Kl. score = 2].

Male and female Charles River rats were given in their diet 0, 0.1, 0.5 or 1% $C_{14\text{-}15}AE_7$ for two years. There were no treatment-related changes in general behavior and appearance. The survival rate of the test animals was comparable if not better than the controls. Body weights of the 0.5% females and the 1% males and females had significantly lower weight gains than the control. There were no treatment-related effects on organ weights and tumor incidence (HERA, 2009) [Kl. score = 2].

Male and female Sprague-Dawley rats were given in their diet $C_{14\text{-}15}AE_7$ at 0.1, 0.5 and 1% for two years. A treatment-related body weight depression was observed in females at the two highest treatment levels and in males at the 1% dose level, probably due to the poor palatability of the diet. There was no evidence for any carcinogenic activity (HERA, 2009) [Kl. score = 2].

H. Reproductive Toxicity

No studies are available on alcohols, C12-16, ethoxylated.

CD rats were given in their diet 0, 0.05, 0.1 or 0.5% (approximately 0, 25, 50 or 250 mg/kg-day) $C_{12}AE_6$ in a two-generation reproductive toxicity study. There were no treatment related effects in the parents or pups on general behavior, appearance or survival. At 0.5%, there was reduced weight gain in both the parental animals and the pups compared to the controls. Fertility was unaffected by treatment. The NOAEL for reproductive toxicity is 0.5% in the diet, which corresponds to 250 mg/kg-day (HERA, 2009) [Kl. score = 2].

In a two-generation developmental and teratogenicity study, CD rats were given in their diet 0, 0.05, 0.1 or 0.5% $C_{14\text{-}15}AE_7$ (approximately 0, 25, 50 or 250 mg/kg-day). Three of the treated groups were given the test substance continuously throughout the study; in the other three groups the females received the test substance on GD 6-15 and the males were untreated. None of the deaths of parental rats during the study was considered to be compound-related. There were no treatment-related changes in behavior or appearance in the parental rats or pups. Slightly lower body weight gain was noted in the 0.5% continuously treated females. Food consumption was similar for control and treated rats. Fertility, gestation and viability indices were similar across groups. The average 21-day body weights for the 0.5% continuous treated pups were significantly lower than that of the control. Relative liver weights of the 0.5% continuously treated F_1 parental animals were increased at the 91-day sacrifice; relative liver weights of the 0.5% continuously treated males were also increased at the 60-day and caesarean section sacrifices. There were no treatment-related histopathological lesions in any of the tissues from the F_0 and F_1 generations. The NOAEL for reproductive toxicity is 0.5% in the diet or 250 mg/kg-day (HERA, 2009) [Kl. score = 2].

I. Developmental Toxicity

No studies are available on alcohols, C12-16, ethoxylated.

In a two-generation reproductive toxicity study, Charles River rats were given in their diet 0, 0.05, 0.1 or 0.5% (about 0, 25, 50 or 250 mg/kg-day) $C_{12}AE_6$. General behavior, appearance and survival were unaffected by treatment. At the 0.5% dose level, adults and pups gained less weight than the control rats. In the 0.5% dose group, there was a statistical increase in embryo lethality and soft tissue anomalies and at the 0.1% there was a statistical decrease in mean fetal liver weight. Neither of these effects was considered to be treatment-related by the authors as they showed no dose response characteristics. The NOAEL for maternal toxicity is 50 mg/kg-day. The NOAEL for developmental and teratogenicity is 0.1% in the diet or 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Pregnant rabbits were given by oral gavage 0, 50, 100 or 200 mg/kg $C_{12}AE$ from gestational days 2 to 16. Nine control rabbits and 31 treated rabbits died during the study. Surviving rabbits at the 200 mg/kg dose group generally showed slight losses of body weight. At 100 and 200 mg/kg, ataxia and a slight decrease in body weight was observed in the pregnant animals. In seven treated and two control rabbits, early deliveries were recorded. There were no treatment-related effects on corpora lutea, implantations, number of live fetuses and spontaneous abortions. The NOAEL for maternal toxicity is 50 mg/kg-day; the NOAEL for developmental toxicity is 200 mg/kg-day (HERA, 2009) [Kl. score = 2].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for alcohols, C12-16, ethoxylated follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Two-year dietary studies in rats have been conducted on alcohol ethoxylates $C_{12\text{-}13}AE_{6.5}$ and $C_{14\text{-}15}AE_{7}$ (HERA, 2009). The lowest NOAEL from these studies is 50 mg/kg-day based on increased organ weights. The NOAEL of 50 mg/kg-day will be used to derive an oral reference dose and drinking water guidance value for alcohols, C12-16, ethoxylated.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:

UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 50/(10 x 10 x 1 x 1 x 1) = 50/100 = 0.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:

Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.5 x 70 x 0.1)/2 = 1.8 mg/L

Cancer

Several alcohol ethoxylates similar to alcohols, C12-16, ethoxylated were not carcinogenic to rats in a two-year dietary study. Thus, a cancer reference value was not derived.

K. HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

Ethoxylated C12-C16 alcohol does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidizing potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

There are no aquatic toxicity studies for ethoxylated C12-C16 alcohol. The aquatic toxicity of other AEs has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. AEs have moderate chronic toxicity to aquatic life.

B. Aquatic Toxicity

Acute Studies

There are no acute aquatic toxicity studies for ethoxylated C12-C16 alcohol. The aquatic toxicity of other AEs has been extensively evaluated in numerous studies on fish, daphnids and algae as well as microorganisms. Table 3 lists the results of acute aquatic toxicity studies on read across substance alcohols, C12-C15, ethoxylated (1 to 2.5 EO) [CAS No. 68131-39-5], alcohols, C12-C14, ethoxylated (2 EO) [CAS No. 68439-50-9] and alcohols, C12-C15, branched and linear, ethoxylated [CAS No. 106232-83-1].

Table 3 Acute Aquatic Toxicity Studies on Ethoxylated C12-C16 Alcohol[a,b,c]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss (Rainbow Trout)	96-hr LC_{50}	1.3 – 1.7[a]	2	ECHA
Danio Rio	96-hr LC_{50}	1.2[b]	2	ECHA
Danio Rio	96-hr LC_{50}	2[b]	2	ECHA
Zebrafish	96-hr LC_{50}	>2[c]	2	ECHA
Daphnia magna	48-hr EC_{50}	0.14[a]	2	ECHA
Daphnia magna	48-hr EC_{50}	0.23[a]	2	ECHA
Daphnia magna	48-hr EC_{50}	0.53[b]	2	ECHA
Daphnia magna	48-hr EC_{50}	2.84[b,d]	2	ECHA
Daphnia magna	48-hr EC_{50}	1.2[e]	1	ECHA
Daphnia magna	48-hr EC_{50}	>2[b]	2	ECHA
Daphnia magna	48-hr EC_{50}	>2[c]	2	ECHA
Daphnia magna	48-hr EC_{50}	0.23	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pseudokirchneriella subcapitata	72-hr EC_{50}	0.75[a]	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	>2[c]	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	0.41[b]	2	ECHA
Desmodesmus subspicatus (green algae)	72-hr EC_{50}	0.778[b]	2	ECHA
Desmodesmus subspicatus (green algae)	72-hr EC_{50}	0.87[e]	1	ECHA
Desmodesmus subspicatus (green algae)	72-hr EC_{50}	1.3[e]	1	ECHA

a: Read across to alcohols, C12-C15, ethoxylated (1 to 2.5 EO) CAS No. 68131-39-5
b: Read across to alcohols, C12-C14, ethoxylated (EO 2) CAS No. 68439-50-9
c: Read across to alcohols, C12-C15, branched and linear, ethoxylated (CAS No. 106232-83-1)
d: alcohols, C12-C14, ethoxylated (EO 1) CAS No. 68439-50-9 as WAF (water accommodated fraction)
e: alcohols, C12-C14, ethoxylated (EO 4 or EO 6) CAS No. 68439-50-9

A review of the acute studies indicates that invertebrates are somewhat more sensitive to AEs than fish and algae. As concluded in HERA (2009), the Danish EPA (2001) found that the acute toxicity of AE to invertebrates varies, with EC50 values from 0.1 mg/l to more than 100 mg/l for linear AE and from 0.5 mg/l to 50 mg/l for branched AE. The toxicity is species specific and may vary between 0.29 mg/l and 270 mg/l for the same linear AE (Lewis and Suprenant 1983, quoted in Danish EPA 2001). The most commonly used invertebrates for testing are Daphnia magna and Daphnia pulex, and they are also among the most sensitive invertebrates to AE. The Danish EPA (2001) found that some AE are very toxic to invertebrates, i.e., linear AE of C12-15 EO1-8 and branched AE with a low degree of branching, i.e. < 10-25%. They concluded that branching of the alkyl chain reduces the toxicity of AE to invertebrates, as also observed for algae (Danish EPA 2001). However, the data used to reach this conclusion is from specially synthesized AE which have been shown to have a significantly higher toxicity than the AE made from a technical alcohol which are used commercially (Kaluza and Taeger, 1996).

Chronic Studies

In developing a water quality guideline for AEs (ANZG, 2018), the toxicity data was normalised for a specific alkyl chain length or a specific number of EO groups. The NOECs listed below were normalised to an alkyl chain length of C13.3 and EO of 8.2. There were chronic data for 13 species that belonged to 7 taxonomic groups (fish, crustacea, blue alga, diatoms, green alga, protozoa, and worms).

Freshwater fish: 2 species, 720 to 1,500 µg/L.

Freshwater crustaceans: 2 species, 590 to 860 µg/L.

Freshwater rotifers: 1 species, *Brachionus calyciflorus*, 1,300 µg/L.

Freshwater algae, diatoms and blue-green algae: 6 species, 200 to 8,700 µg/L.

Freshwater mesocosms: 4 NOEC data for multiple species tests were 80, 80, 320 and 330 µg/L, although replication was insufficient to meet OECD (1992) requirements. Normalised data were 380, 380, 320 and 1,520 µg/L.

C. Terrestrial Toxicity

No studies are available. The substance is readily biodegradable. Therefore, soil is not expected to be a compartment of concern. Thus, the risk to terrestrial macroorganisms is regarded to be negligible (ECHA).

D. Calculation of PNEC

The PNEC calculations for ethoxylated C12-C16 alcohol follow the methodology discussed in DEWHA (2009).

PNEC water

The ANZG water quality guideline (2018) in freshwater is: "A high reliability trigger value of 140 µg/L was derived for AE (normalized data) using the statistical distribution method with 95% protection."

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Nonetheless, a $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.0875 mg/kg sediment wet weight.

The calculations are as follows:
$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 0.800/1280 \times 1000 \times 0.140$
$= 0.0875$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = 0.002 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 156.8)/1000 \times 2400]$
$= 0.800\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]

$Kp_{sed} = K_{oc} \times f_{oc}$
= 3920 x 0.04
= 156.8 L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for alcohols, C12-16, ethoxylated based on the molecular connectivity index (MCI) is 3,920 L/kg (USEPA, 2018).
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 7.32 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
= (78.4/1500) x 1000 x 0.14
= 7.32mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 kg/m^3 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
= 3920 x 0.02
= 78.4 m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for alcohols, C12-16, ethoxylated based on the molecular connectivity index (MCI) is 3,920 L/kg (USEPA, 2018).
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Ethoxylated C12-C16 alcohol is readily biodegradable and thus does not meet the screening criteria for persistence.

The bioconcentration factors (BCF) in fish for ethoxylated alcohols (which includes ethoxylated C12-C16 alcohol) have been reported to range from <5 to 387.5. Thus, ethoxylated C12-C16 alcohol does not meet the screening criteria for bioaccumulation.

The chronic NOEC values for alcohols ethoxylates are >0.1 mg/L. Thus, ethoxylated C12-C16 alcohol do not meet the criteria for toxicity.

Thus, ethoxylated C12-C16 alcohol is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for ethoxylated C12-C16 alcohol.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Alcohols, C12-16, ethoxylated	68551-12-2	Not a PBT	No	No	No	No	No	No	2 (fish), 3 (inv and algae)	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework). Acute aquatic toxicity for invertebrates and algae range between 0.14 and 2.84 mg/L with variability likely due to varying test conditions and differences in chemical structure.
3 – Tier 2 – Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AE	alcohol ethoxylates
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Environment Guidelines
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EO	ethoxylate
EU	European Union
g/cm^3	grams per cubic centimetre
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
MCI	molecular connectivity index
mg/L	milligrams per litre
mPA s	millipascal second
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
					0	30	0	30	0	30	
Alcohols, C12-16, ethoxylated	68551-12-2	1.50E+00	1.50E+01	2.00E-01	2.00E-02	5.00E-03	2.00E-04	5.00E-05	4.00E-06	1.00E-06	1.40E-01

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Ethyl Hexanol

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Ethyl hexanol is a component in a product used in the KCl/Polymer Stuck Pipe Mud system. The secondary mud system is used to free stuck pipes and, as a secondary mud, will only be used as required. As a result, these secondary muds are considered insignificant relative to the primary muds due to the considerably reduced volume used (<0.1%) as compared to the other muds.

The purpose and maximum quantity (i.e., in all muds) for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Ethyl hexanol	104-76-7	Lubricant	NA

[1] Based on maximum of combined muds assessed.
CAS No = Chemical Abstracts Service Number
NA = quantity used varies with severity of loss

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on ethyl hexanol, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Ethyl hexanol (104-76-7)	2-yr rat oral gavage	Reduced body weight, clinical signs	50	100	0.5	2

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 presents the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Ethyl hexanol (104-76-7)	Acute *Daphnia*	11.5	1,000	0.012

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Ethyl hexanol (104-76-7)	[a]	-	-	0.027

[a]Calculated using equilibrium partitioning method.
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Ethyl hexanol (104-76-7)	[a]	-	-	0.017

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Ethyl hexanol is a clear and colourless liquid. The molecular structure of ethyl hexanol is presented in **Figure 1**.

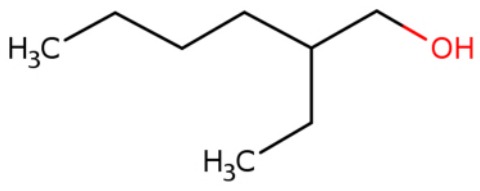

Figure 1 Molecular Structure of Ethyl Hexanol[2]

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/104-76-7

2-Ethylhexanol is readily biodegradable. It is not expected to bioaccumulate. 2-Ethylhexanol has a low tendency to bind to soil or sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for ethyl hexanol is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that ethyl hexanol is not a PBT substance.

Human Health Hazards

Ethyl hexanol has low acute toxicity by the oral route; virtually no acute toxicity by the dermal route; and, has moderate acute toxicity by the inhalation route. It is a skin and eye irritant. No skin sensitisation studies on ethyl hexanol were located.

Repeated exposure studies in rodents caused liver effects (i.e., peroxisomal proliferation); these effects are not thought to occur in humans. Ethyl hexanol is not expected to have an effect on reproduction based on findings in animals from similar compounds. No developmental toxicity was seen in animals exposed to ethyl hexanol by the oral, dermal or inhalation routes. Ethyl hexanol is not genotoxic or carcinogenic.

Based on a review of a two-year chronic oral study in rats and mice, TRVs were derived for ethyl hexanol. The drinking water guideline value derived for ethyl hexanol using the non-carcinogenic oral RfD is 1.75 mg/L (or 2 mg/L) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Ethyl hexanol may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to ethyl hexanol in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in recovered drilling fluids would be diluted by at least 90% in the water feed pond due to the aggregation with produced water. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, ethyl hexanol is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, ethyl hexanol is moderately toxic to aquatic organisms. Acute toxicity towards algae, fish and aquatic invertebrates is of the same order of magnitude. However, *Daphnia magna* was of somewhat less sensitivity compared to fish and algae (ECHA).

Ethyl hexanol is readily biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for ethyl hexanol are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs in water. However, there are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of ethyl hexanol in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of ethyl hexanol in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as ethyl hexanol, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

ETHYL HEXANOL
[2-ETHYLHEXANOL]

This dossier on ethyl hexanol (designated in this dossier as 2-ethylhexanol) presents the most critical studies pertinent to the risk assessment of ethyl hexanol in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Ethyl hexanol was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Ethyl hexanol was assessed as a tier 2 chemical for acute toxicity and chronic toxicity. Therefore, ethyl hexanol is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

2-Ethylhexanol is readily biodegradable, and it is not expected to bioaccumulate. 2-Ethylhexanol has a low tendency to bind to soil or sediment. 2-Ethylhexanol has low acute toxicity by the oral route; virtually no acute toxicity by the dermal route; and has moderate acute toxicity by the inhalation route. It is a skin and eye irritant. No skin sensitisation studies on 2-ethylhexanol were located. Repeated exposure studies in rodents causes liver effects (i.e., peroxisomal proliferation); these effects are not thought to occur in humans. 2-Ethylhexanol is not genotoxic. Lifetime oral studies in rats and mice showed no carcinogenic effects. 2-Ethylhexanol is not expected to cause reproductive toxicity based on findings in animals from similar compounds. No developmental toxicity was seen in animals exposed to 2-ethylhexanol by the oral, dermal or inhalation routes. 2-Ethylhexanol is of moderate toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-Ethylhexan-1-ol

CAS RN: 104-76-7

Molecular formula: $C_8H_{18}O$

Molecular weight: 130.23 g/mol

Synonyms: 2-Ethylhexanol, 2-ethylhexan-1-ol, 2-ethyl-*n*-hexyl alcohol

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of 2-Ethylhexanol

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear and colourless liquid	2	ECHA
Melting Point	-89°C @ 101.kPa	2	ECHA
Boiling Point	185°C @ 101.3 kPa	2	ECHA
Density	833 kg/m^3 @ 20°C	2	ECHA
Vapor Pressure	93 Pa @ 20°C 120 Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	2.9 @ 25°C	2	ECHA
Water Solubility	0.9 g/L @ 20°C	2	ECHA
Dissociation Constant (pKa)	15.75@ 25°C	2	ECHA
Viscosity	9.7 mPa s @ 20°C 4.3 mPa s @ 40°C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for 2-ethylhexanol.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

2-Ethylhexanol is readily biodegradable. It is not expected to bioaccumulate. 2-Ethylhexanol has a low tendency to bind to soil or sediment.

B. Partitioning

2-Ethylhexanol is slightly soluble in water. Based upon a Henry's Law constant of 2.6 Pa*m³/mol, it is expected to volatilise from water and moist soil surfaces. However, it is not expected to volatilise from dry soil surfaces based upon its vapour pressure. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions (pH 5 to 9) (PubChem).

C. Biodegradation

2-Ethylhexanol was considered readily biodegradable in an OECD TG 301C test. After two weeks, degradation was 79 to 99.9% measured by O_2 consumption, 100% degradation measured by TOC removal and 100% degradation as determined by test material analysis (ECHA) [Kl score = 1]. 2-Ethylhexanol was inherently biodegradable in a Zahn-Wellens test (OECD TG 302B), with >95% degradation within five days (ECHA). [Kl. score = 2]

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental data are available for 2-ethylhexanol. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 105.6 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 35.28 L/kg. Based upon these K_{oc} values, if released to soil, 2-ethylhexanol is expected to have high to very high mobility. If released into water, based on these K_{oc} values and Henry's Law constant, 2-ethylhexanol is not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

No bioconcentration studies have been conducted on 2-ethylhexanol. Per calculations using EPISuite™ (USEPA, 2017), the log BCF via the Arnot-Gobas method for upper trophic level organisms is 1.543 (BCF = 34.88). Thus, 2-ethylhexanol is not expected to bioaccumulate, which is consistent with its experimental log K_{ow} of 2.9 (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

2-Ethylhexanol has low acute toxicity by the oral route; virtually no acute toxicity by the dermal route; and has moderate acute toxicity by the inhalation route. It is a skin and eye irritant, but not a skin sensitiser. Repeated exposure studies in rodents caused liver effects (*i.e.*, peroxisomal proliferation); these effects are not thought to occur in humans. 2-Ethylhexanol is not genotoxic.

Lifetime oral studies in rats and mice showed no carcinogenic effects. 2-Ethylhexanol is not expected to have an effect on reproduction based on findings in animals from similar compounds. No developmental toxicity was seen in animals exposed to 2-ethylhexanol by the oral, dermal or inhalation routes.

B. Acute Toxicity

The oral LD_{50} values in rats are: 2,047 mg/kg (Smyth et al., 1969); 3,290 mg/kg (Schmidt et al., 1973); and 3,730 mg/kg (Scala and Burtis, 1973). [Kl. scores = 2]

The 4-hour whole body inhalation LC_{50} in rats is >890 mg/m^3; no deaths were reported (ECHA). [Kl. score 2]

The dermal LD_{50} values in rats and rabbits are >3,000 and >2,600 mg/kg, respectively. There were no deaths in either study (ECHA). [Kl. score = 1 and 2, respectively]

C. Irritation

Application of 0.5 mL 2-ethylhexanol to the skin of rabbits for 4 hours under semi-occlusive conditions was severely irritating (ECHA). [Kl. score = 1]

Instillation of 0.1 mL 2-ethylhexanol into the eyes of rabbits was irritating. The mean of the 24, 48 and 72 hours scores were: 1.44 for corneal opacity; 0.89 for iridial lesions; 2.56 for conjunctival redness; and 0.78 for chemosis. The effects were fully reversible within 21 days (ECHA). [Kl. score = 1]

D. Sensitisation

2-Ethylhexanol lacks skin sensitizing properties. In an experimental skin sensitisation study with 29 human volunteers using the maximization method of Kligman, no skin sensitisation was seen in any of the 29 test subjects (ECHA). [Kl. Score = 3]

No valid respiratory sensitisation studies are available.

E. Repeated Dose Toxicity

<u>Oral</u>

Male F344 rats were given in their feed 0 or 2% 2-ethylhexanol for three weeks. The objective of this study was to investigate the liver effects of 2-ethylhexanol on hepatic peroxisome proliferation and peroxisome enzymes. There were no significant treatment-related effects on body weight, but liver weights relative to body weights, catalase activity, liver carnitine acetyltransferase activity, and hepatic peroxisome proliferation (as determined by electron microscopy) were significantly increased. There was also a treatment-related decrease on serum levels of cholesterol and triglycerides. The LOAEL is 2% in the diet; a NOAEL was not established (Moody and Reddy, 1978). [Kl. score = 2]

Male and female F344 rats were dosed with 0, 25, 125, 250 or 500 mg/kg 2-ethylhexanol (in an aqueous suspension with an emulsifier) 5 days/week for 13 weeks. Body weights were decreased in

the 500 mg/kg group (both sexes). Relative liver, kidney and stomach weights were increased in the 250 and 500 mg/kg groups. Gross pathological examination showed forestomach lesions in the 500 mg/kg animals. Palmitoyl CoA oxidase activity was increased in the livers of the 500 mg/kg animals (both sexes). The NOAEL for systemic toxicity is 125 mg/kg-day (Astill *et al.*, 1996a). [Kl score = 1]

Male and female B6C3F_1 mice were dosed with 0, 25, 125, 250 or 500 mg/kg 2-ethylhexanol (in an aqueous suspension with an emulsifier) 5 days/week for 13 weeks. Treatment-related effects included increased stomach weights (≥250 mg/kg) and increased liver weights (125 and 250 mg/kg, respectively). Treatment-related histopathological changes were limited to acanthosis (diffuse hypertrophy or thickening of the prickle cell layer) of the forestomach mucosa in the 500 mg/kg animals (both sexes). No increases in palmitoyl CoA oxidase activity were seen in the livers of male and female mice at any dose level. The NOAEL for systemic toxicity is 500 mg/kg-day (Astill *et al.*, 1996a). [Kl. score = 1]

Male and female F344 rats were dosed by oral gavage with 0, 50, 150 or 500 mg/kg 2-ethylhexanol (in 0.0005% Cremophor EL, a polyoxyl-35 castor oil) 5 days/week for two years. A water control was also included in the study. There were no differences of biological importance between the vehicle control and a water control group. Reduced body weight gain occurred in the 150 and 500 mg/kg groups with an increased incidence of lethargy and unkemptness. There were dose-related increases in relative liver, stomach, brain, kidney and testis weights at study termination. Mortality was significantly increased among the 500 mg/kg females, and there was marked aspiration-induced bronchopneumonia in the high-dose animals. Gross and histopathological non-neoplastic changes were similar between treated and control groups. The NOAEL is 50 mg/kg-day (Astill *et al.*, 1996b). [Kl. score = 1]

Male and female B6C3F_1 mice were dosed by oral gavage with 0, 50, 200 or 750 mg/kg 2-ethylhexanol (in 0.0005% Cremophor EL, a polyoxyl-35 castor oil) 5 days/week for two years. A water control was also included in the study. There were no differences of biological importance between the vehicle control and a water control group that was also included in the study. All treatment-related effects occurred only in the 750 mg/kg animals (both sexes). Mortality was increased and body weight gain was reduced, and there was a slight increase in nonneoplastic focal hyperplasia in the forestomach. Relative liver and stomach weights occurred in the 750 mg/kg animals (both sexes). The NOAEL is 200 mg/kg-day (Astill *et al.*, 1996b). [Kl. score = 1]

Inhalation

Male and female Wistar rats were exposed by inhalation (whole body exposure) to 0, 15, 40 or 120 ppm 2-ethylhexanol 6 hours/day, 5 days/week for 13 weeks. No adverse effects including cyanide-insensitive palmitoyl CoA oxidation (a parameter for hepatic peroxisome proliferation) were observed. The NOAEC for this study is 120 ppm (ECHA). [Kl. score = 1]

Dermal

No adequately or reliable studies are available.

F. Genotoxicity

In Vitro Studies

The results of the *in vitro* genotoxicity studies on 2-ethylhexanol are presented in Table 3.

Table 3 *In Vitro* Genotoxicity Studies on 2-Ethylhexanol

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* and *E. coli* strains)	-	-	1	ECHA
Mammalian cell gene mutation (CHO cells/HGPRT)	-	-	1	ECHA
Mammalian cell gene mutation (L5178Y mouse lymphoma cells)	-	-	1	ECHA
Chromosomal aberration (CHO cells)	-	-	2	ECHA
Sister chromatid exchange (CHO cells)	-	-	2	ECHA

*+, positive; -, negative

In Vivo Studies

Male and female B6C3F_1 mice were given 456 mg/kg 2-ethylhexanol either as single intraperitoneal injection or two intraperitoneal injections on two consecutive days. There were no increases in micronuclei in the bone marrow polychromatic erythrocytes under either dosing regimen (ECHA). [Kl. score = 2]

G. Carcinogenicity

Oral

Male and female F344 rats were dosed by oral gavage with 0, 50, 150 or 500 mg/kg 2-ethylhexanol (in 0.0005% Cremophor EL, a polyoxyl-35 castor oil) 5 days/week for two years. A water control was also included in the study. There was no evidence of treatment-related neoplastic lesions in any of the exposed groups (Astill *et al.*, 1996b). [Kl. score = 1]

Male and female F344 rats were dosed by oral gavage with 0, 50, 200 or 750 mg/kg 2-ethylhexanol (in 0.0005% Cremophor EL, a polyoxyl-35 castor oil) 5 days/week for two years. A water control was also included in the study. There was a 12% incidence of hepatic basophilic foci and an 18% incidence of liver carcinomas in the 750 mg/kg male mice, which was not statistically significant compared with either control by Fisher's exact test. There was a 12% incidence of hepatic basophilic foci and a 10% incidence of liver carcinomas in the 750 mg/kg female mice, which was statistically significant compared with the vehicle but not with the water controls by Fisher's exact test. There was a weak trend in hepatocellular carcinoma incidence in the 750 mg/kg dose group, which may have been associated with toxicity. The time-adjusted incidence of hepatocellular carcinomas in male mice (18.8%) was within the historical control range at the testing facility (0–22%), but was outside the normal range of 0–2% for the female mice (13.1%) (Astill *et al.*, 1996b). [Kl. score = 1]

Inhalation

No studies are available.

H. Reproductive Toxicity

There are no reproductive toxicity studies on 2-ethylhexanol. However, a two-generation reproductive toxicity study has been conducted on the surrogate di (2-ethylhexyl) terephthalate at dietary doses of 0, 3,000, 6,000 or 10,000 ppm. Di (2-ethylhexyl) terephthalate is expected to be hydrolysed in the body by carboxylesterases to 2-ethylhexanol and terephthalic acid. There were no adverse effects on reproductive parameters that included estrous cyclicity, gonadal functions, spermatogenic endpoints (motility, morphology, counts), mating behaviour and performance, conception, gestation and parturition, and fertility in general. There were no adverse effects noted in the reproductive organs. Reduced postnatal pup weights (potentially related to maternal toxicity) were observed for both sexes in both generations in the 6,000 and 10,000 ppm dose groups. The NOAELs for reproductive and developmental toxicity are 10,000 ppm (the highest dose tested) and 3,000 ppm, respectively (Faber *et al.*, 2007; ECHA). [Kl. score = 2]

I. Developmental Toxicity

Oral

Pregnant female CD-1 mice were given 2-ethylhexanol in their diet by microencapsulation at 0, 0.009, 0.03 or 0.09% on gestational days 0 to 17. The calculated consumption of 2-ethylhexanol based on food consumption was 0, 17, 59 and 191 mg/kg-day, respectively. No maternal or developmental toxicity was observed. The NOAEL for maternal and developmental toxicity is 191 mg/kg-day (ECHA). [Kl. score = 1]

Inhalation

Pregnant female SD rats were exposed by inhalation to 0 or 850 mg/m^3 (approximately 190 ppm) 2-ethylhexanol 7 hours/day during gestational days 1 to 19. The inhalation exposure was considered to be the highest attainable vapor concentration. The only effect seen in the dams was a slight reduction in feed consumption. No developmental toxicity was observed. The NOAEC for maternal and developmental toxicity is 850 mg/m^3 (Nelson *et al.*, 1989; ECHA).

Dermal

Pregnant female F344 rats were given dermal applications of 0, 252, 840 or 2,520 mg/kg 2-ethylhexanol 6 hours/day during gestational days 6 to 15. The only effects seen in the dams were reduced body weight gain in the high-dose group and local skin irritation in the mid- and high-dose groups. No developmental toxicity was observed. The NOAELs for maternal (systemic) and developmental toxicity were 840 and 2,520 mg/kg-day, respectively (Tyl *et al.*, 1992).

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for 2-ethylhexanol follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

Two-year chronic studies have been conducted in rats and mice given oral gavage doses of 2-ethylhexanol. The lowest NOAEL from these studies is 50 mg/kg-day, based on reduced body weight and clinical signs in rats dosed with 150 and 500 mg/kg-day 2-ethylhexanol. The NOAEL of 50 mg/kg-day will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 50/(10 x 10 x 1 x 1 x 1) = 50/100 = 0.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.5 x 70 x 0.1)/2 = 1.75 mg/L

Cancer

2-Ethylhexanol was not carcinogenic to rats or mice in chronic oral studies. Therefore, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

2-Ethylhexanol does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

2-Ethylhexanol is moderately toxic to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on 2-ethylhexanol.

Table 4 Acute Aquatic Toxicity Studies on 2-Ethylhexanol

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Fathead minnow	96-hour LC_{50}	28.2	1	ECHA
Golden Orfe	96-hour LC_{50}	17.1	1	ECHA
Daphnia magna	48-hour EC_{50}	39	2	ECHA
Scenedesmus subspicatus	72-hour EC_{50} EC_{10}	11.5 (biomass) 16.6 (growth rate) 3.2 (biomass) 5.3 (growth rate)	2	ECHA

Chronic Studies

The 72-hour EC_{10} from an algal study using *Scenedesmus subspicatus* was 3.2 and 5.3 mg/L, based on biomass and growth rate, respectively (ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for 2-ethylhexanol follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (17.1 mg/L), invertebrates (39 mg/L) and plants (11.5 mg/L). On the basis that the data consists of short-term studies from three trophic levels, an assessment factor of 1,000 has been applied to the lowest reported EC_{50} value of 11.5 mg/L for algae. The $PNEC_{water}$ is 0.012 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.027 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (2.83/1280) \times 1000 \times 0.012$
$= 0.019$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water (mg/L) [calculated above]

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 4.22/1000 \times 2400]$
$= 2.83\ m^3/m^3$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 105.6 \times 0.04$
$= 4.22$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for 2-ethylhexanol calculated from EPISuite™ using log K_{ow} is 105.6 L/kg .
f_{oc} = fraction of organic carbon in sediment = 0.04 [default]

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.017 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (2.11/1500) \times 1000 \times 0.012$
$= 0.017$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water (mg/L) [calculated above]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 105.6 \times 0.02$
$= 2.11\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for 2-ethylhexanol calculated from EPISuite™ using log K_{ow} is 105.6 L/kg .
f_{oc} = fraction of organic carbon in soil = 0.02 [default]

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

2-Ethylhexanol is readily biodegradable; thus it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of 2.9, 2-ethylhexanol does not meet the screening criteria for bioaccumulation.

The 72-hour EC_{10} from an algal study on 2-ethylhexanol is >0.1 mg/L. The acute EC_{50} for 2-ethylhexanol in fish, invertebrates and algae are >1 mg/L. Thus, 2-ethylhexanol does not meet the screening criteria for toxicity.

Therefore, 2-ethylhexanol is not a PBT substance.**Other Characteristics of Concern**

No other characteristics of concern were identified for 2-ethylhexanol.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity [2]	
2-Ethylhexanol	104-76-7	Not a PBT	No	No	No	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
CHO	Chinese hamster ovary
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HGPRT	Hypoxanthine-guanine phosphoribosyltransferase
HHRA	enHealth Human Risk Assessment
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system

KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEC	No Observed Adverse Effect Concentration
NOAEL	no observed adverse effect level
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
TOC	total organic carbon
USEPA	United States Environmental Protection Agency

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
Ethyl hexanol	104-76-7	6.70E+01	1.50E+01	6.70E+00	1.68E+00	6.70E-02	1.68E-02	1.34E-03	3.35E-04	1.20E-02

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Hydrogen Peroxide

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Hydrogen peroxide is a component in a Water Management Facility (WMF) product used for membrane cleaning during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Hydrogen peroxide	7722-84-1	Membrane cleaning	2 x 1000 L (IBC)
Acetic Acid	64-19-7		
Peroyxacetic Acid	79-21-0		
Water	7732-18-5		

CAS No = Chemical Abstracts Service Number
IBC = intermediate bulk container
L = litre

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Hydrogen peroxide is not a carcinogen; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Hydrogen peroxide (7722-84-1)	90-day rat drinking water	Reduced body weights, food consumption; duodenal hyperplasia	239	300	1.0	3.5

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 2** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to **Attachment 2** and the dossier regarding the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Hydrogen peroxide (7722-84-1)	Chronic *Daphnia* and algae	0.63	50	0.013

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Hydrogen peroxide is a naturally occurring chemical, and is produced by almost all cells as a part of normal metabolic processes (OECD, 1999). Hydrogen peroxide is normally handled as an aqueous solution. Commercial solutions must be stabilised with additives to prevent possible violent decomposition due to catalytic impurities or elevated temperatures and pressure (EU, 2003). Hydrogen peroxide is used widely as an oxidising and a reducing agent. The molecular structure of hydrogen peroxide is presented in **Figure 1**.

Figure 1 Molecular Structure of Hydrogen Peroxide[2]

Hydrogen peroxide is normally a short-lived substance in the environment. It is biologically degraded by an enzyme-mediated process, which is rapid and can be considered equivalent to readily biodegradable. Abiotic degradation of hydrogen peroxide is also an important process, involving transition metals, reaction with itself, organic compounds that can react with hydrogen peroxide and other factors such as heat and sunlight. Hydrogen peroxide is not expected to bioaccumulate because it is a reactive polar substance.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for hydrogen peroxide is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that hydrogen peroxide is not a PBT substance.

Human Health Hazards

Hydrogen peroxide has moderate acute toxicity by the oral and inhalation routes and low acute toxicity by the dermal route. Depending on the concentration, solutions of hydrogen peroxide are corrosive, irritating or non-irritating. These solutions cause direct effects to the skin, eyes, respiratory tract and gastrointestinal tract. Vapours from aqueous solutions of hydrogen peroxide can cause respiratory irritation. Hydrogen peroxide is not a skin sensitiser.

Repeated oral doses of a hydrogen peroxide solution in drinking water resulted in mucosal hyperplasia of the duodenum (small intestine) in male and female rats; no other effects were seen in the gastrointestinal tract or in other organs. Repeated inhalation exposures to hydrogen peroxide resulted in an inflammatory response in the larynx of male and female rats but not in any other locations of the respiratory tract, including the lung. In vitro genotoxicity tests have shown positive responses with hydrogen peroxide; however, in vivo studies are negative for genotoxicity. There are no adequate carcinogenicity, reproductive or developmental toxicity studies on hydrogen peroxide.

[2] Source https://pubchem.ncbi.nlm.nih.gov/compound/784#section=2D-Structure

Based on a review of repeated dose toxicity studies, TRVs were derived for hydrogen peroxide. The drinking water guideline value derived for hydrogen peroxide using the non-carcinogenic oral RfD is 3.5 mg/L (see **Table 2**). A detailed discussion of the drinking water guideline values is presented in **Attachment 2**.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents. Based on the treatment process described in **Attachment 1**, membrane cleaning waste is directed to the brine dams where hydrogen peroxide will rapidly break down. As a result, this chemical would not be present in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

Hydrogen peroxide is moderately toxic to aquatic organisms on an acute and chronic basis. However, all aerobic aquatic organisms are naturally adapted to fluctuating background concentrations of hydrogen peroxide in natural waters (NICNAS, 2017).

Hydrogen peroxide is readily biodegradable and does not persist in the environment. Abiotic degradation of hydrogen peroxide is also an important process. The chemical also does not bioaccumulate.

Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs (see **Table 3**). However, no experimental toxicity data on sediment or soil organisms are available. Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics, such as hydrogen peroxide. Thus, the equilibrium partitioning method cannot be used to calculate PNECs for soil or sediment. Based on its properties, hydrogen peroxide is not expected to significantly adsorb to sediment or soil, and the assessment of this compartment will be covered by the aquatic assessment. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 2**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point, including the following
- Livestock and wildlife that may access Dawson River surface water

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with the following Matters of National Environmental Significance [MNES] receptors:

- White-throated Snapping Turtle (*Elseya albagula*) – Critically endangered; and
- Fitzroy River Turtle (*Rheodytes leukops*) – Vulnerable.

These findings are consistent with an assessment completed by NICNAS in 2017. Based on an assessment of environmental hazards, NICNAS identified hydrogen peroxide as a chemical of low

concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

References

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NICNAS. (2017). National assessment of chemicals associated with coal seam gas extraction in Australia,Technical report number 14 - Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

OECD. (1999). SIDS initial assessment profile: hydrogen peroxide, Organisation for Economic Cooperation and Development, Paris, France.

Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration	
Hydrex 4714 (CIP)	Hydrogen Peroxide Acetic Acid Peroxyacetic Acid Water	7722-84-1 64-19-7 79-21-0 7732-18-5	20-30% 10-20% 5-10% NA	Hydrex 4714	Veolia Water Solutions	Reverse Osmosis Plant	1000L IBC		2 x 1000L (IBC)		NIL		NIL

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Purpose / Function	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation
					(mg/L)	Permeate notes	(mg/kg)	(mg/kg)
Hydrex 4714 (CIP)	Hydrogen Peroxide	7722-84-1	membrane cleaning	Membrane cleaning waste is directed to the Brine Dams	NA	This product is not directed to the permeate stream.	NA	NA
	Acetic Acid	64-19-7			NA	This product is not directed to the permeate stream.	NA	NA
	Peroxyacetic Acid	79-21-0			NA	This product is not directed to the permeate stream.	NA	NA
	Water	7732-18-5			NA	This product is not directed to the permeate stream.	NA	NA

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Concentration	
			(mg/L)	Brine Notes
Hydrex 4714 (CIP)	Hydrogen Peroxide	7722-84-1	NA	all compounds break down, end up with water and carbon dioxide
	Acetic Acid Peroxyacetic Acid	64-19-7 79-21-0	NA	will biodgrade with in pond
	Water	7732-18-5	NA	

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

HYDROGEN PEROXIDE

This dossier on hydrogen peroxide presents the most critical studies pertinent to the risk assessment of hydrogen peroxide in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Hydrogen peroxide was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Hydrogen peroxide was assessed as a tier 2 chemical for acute toxicity and as a tier 3 chemical based on a limited single chronic study. Therefore, hydrogen peroxide is classified overall as a **tier 2** chemical based on the preponderance of data and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Hydrogen peroxide is a strong oxidising liquid. Hydrogen peroxide is normally a short-lived substance in the environment. It is biologically degraded by an enzyme-mediated process, which is rapid and can be considered equivalent to readily biodegradable. Abiotic degradation of hydrogen peroxide is also an important process, involving transition metals, reaction with itself, organic compounds that can react with hydrogen peroxide and other factors such as heat and sunlight.

Hydrogen peroxide has moderate acute toxicity by the oral and inhalation routes and low acute toxicity by the dermal route. Depending on the concentration, solutions of hydrogen peroxide are corrosive, irritating or non-irritating. These solutions cause direct effects to the skin, eyes, respiratory tract and gastrointestinal tract. Vapours from aqueous solutions of hydrogen peroxide can cause respiratory irritation. Hydrogen peroxide is not a skin sensitiser. Repeated oral doses of a hydrogen peroxide solution in drinking water resulted in mucosal hyperplasia of the duodenum (small intestine) in male and female rats; no other effects were seen in the gastrointestinal tract or in other organs. Repeated inhalation exposures to hydrogen peroxide resulted in an inflammatory response in the larynx of male and female rats but not in any other locations of the respiratory tract, including the lung. In vitro genotoxicity tests have shown positive responses with hydrogen peroxide; however, in vivo studies are negative for genotoxicity. There are no adequate carcinogenicity, reproductive or developmental toxicity studies on hydrogen peroxide. Hydrogen peroxide is moderately toxic to aquatic organisms on an acute and chronic basis.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Hydrogen peroxide
CAS RN: 7722-84-1
Molecular formula: H_2O_2
Molecular weight: 34.0 g/mol

Synonyms: Hydrogen peroxide; hydrogen dioxide; dihydrogen dioxide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Hydrogen Peroxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless, clear liquid without odour	1	EU, 2015
Melting Point	-0.43°C (pure H_2O_2) (pressure not provided)	2	EU, 2015
Boiling Point	150°C @ 101.3 kPa	2	EU, 2015
Density	1,710 kg/m^3 @ -20°C (pure H_2O_2) 1,290 kg/m^3 @ 20°C (70% soln) 1,200 kg/m^3 @ 20°C (50% soln)	2	EU, 2003
Vapor Pressure	260 Pa @ 25°C (pure H_2O_2) 200 Pa @ 30°C (70% soln) 99 Pa @ 30°C (50% soln)	2	EU, 2003
Partition Coefficient (log K_{ow})	-1.57 (QSAR) (pH and temperature not provided)	2	EU, 2015
Water Solubility	"Miscible in all proportions"	2	EU, 2015
pK_a	11.62 @ 25°C	2	EU, 2015
Viscosity	1.249 mPa/s (pure H_2O_2)	2	EU, 2015

Hydrogen peroxide is normally handled as an aqueous solution. Commercial solutions must be stabilised with additives to prevent possible violent decomposition due to catalytic impurities or elevated temperatures and pressure (EU, 2003).

Hydrogen peroxide can decompose explosively. At atmospheric pressures, vapours containing ≥26 mol% can be exploded by a spark, by contact with catalytically active materials initially at room temperature or by "non-catalytic" materials at elevated temperatures. Because of the high relative volatility of water to hydrogen peroxide, the danger of vapor phase explosion on storage of liquid hydrogen peroxide will be encountered only at >74% solutions at elevated temperatures. At >86 wt%, the liquid can be made to explode (EU, 2003)

Hydrogen peroxide is used widely as an oxidising and a reducing agent.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for hydrogen peroxide.

Based on an assessment of environmental hazards, NICNAS identified hydrogen peroxide as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Hydrogen peroxide is normally a short-lived substance in the environment. It is biologically degraded by an enzyme-mediated process, which is rapid and can be considered equivalent to readily biodegradable. Abiotic degradation of hydrogen peroxide is also an important process, involving transition metals, reaction with itself, organic compounds that can react with hydrogen peroxide and other factors such as heat and sunlight.

B. Partitioning

Hydrogen peroxide decomposes into water and oxygen at rates which depend on contact with catalytic materials, such as metals (transition and heavy), activated carbon and enzymes; and other factors, such as heat and sunlight (EU, 2003).

Pure aqueous solutions of hydrogen peroxide are relatively stable. Stability increases with increasing concentration. Stability of pure hydrogen peroxide in pure water is pH-dependent. Decomposition is acid and alkali induced. Stability is at a maximum at pH 3.5 to 4.5 and decomposition rates are highest in alkaline solution (EU, 2003)

Hydrogen peroxide may react as an oxidant, as a reductant or form additional compounds. Hydrogen peroxide does react easily with various functional groups. Most aromatic and aliphatic amines, as well as most aldehydes, do react with hydrogen peroxide. Hydrogen peroxide reacts with many organic acids to form peracids. Peracid formation in the aquatic environment is an equilibrium reaction (EU, 2003).

C. Biodegradation

Hydrogen peroxide is biologically degradable. The catalase enzyme that metabolises hydrogen peroxide to water and oxygen is found in most aerobic bacteria. Degradation is initiated when hydrogen peroxide comes in contact with microbial material (EU, 2003).

Hydrogen peroxide was tested in a respiration inhibition test (OECD 209) using activated sludge from a primarily domestic wastewater treatment plant. This test was used for hydrogen peroxide since the standard biodegradation tests cannot be used for inorganic substances. Rapid, biologically mediated decomposition of hydrogen peroxide was found in municipal sewage sludge, with a half-life of $\leq$2 minutes. These results would suggest that hydrogen peroxide should be classified as readily biodegradable, fulfilling the 10-day window (ECHA). [Kl. score = 2]

The biodegradation rates of hydrogen peroxide have been studied in natural waters. The summertime degradation rate of hydrogen peroxide was studied in lake water from Ontario, Canada. The half-life of hydrogen peroxide was 7.8 hours for unfiltered lake water. It was determined using different filter sizes that the fraction containing picoplankton was responsible for the major proportion of the biological agent responsible for the degradation of hydrogen peroxide (EU, 2003). Half-lives of between 14.7 and 21.6 hours were measured for hydrogen peroxide in Lake Ontario water. It was determined that bacteria and/or algae were the major agents for the decline in hydrogen peroxide concentrations (EU, 2003).

Hydrogen peroxide is a short-lived substance in soil. Rapid degradation will occur due to high concentration of catalytic material, such as metals, enzymes, easily oxidised/reduced organic substances and living microbes (EU, 2003). The decomposition rate of hydrogen peroxide was found to be first-order with a half-life of four hours in a test using soil from a contaminated site (ECHA).

D. Environmental Distribution

Hydrogen peroxide is unstable and breaks down rapidly to oxygen and water. Therefore, adsorption to soil or sediments or volatilisation from soil or water surfaces are not important environmental fate processes (PubChem).

E. Bioaccumulation

Hydrogen peroxide is not expected to bioaccumulate because it is a reactive polar substance. The logarithmic octanol-water partition coefficient (log K_{ow}) is <-1 indicating no potential for bioaccumulation.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Hydrogen peroxide has moderate acute toxicity by the oral and inhalation routes and low acute toxicity by the dermal route. Depending on the concentration, solutions of hydrogen peroxide are corrosive, irritating or non-irritating. These solutions cause direct effects to the skin, eyes, respiratory tract and gastrointestinal tract. Vapours from aqueous solutions of hydrogen peroxide can cause respiratory irritation. Hydrogen peroxide is not a skin sensitiser. Repeated oral doses of a hydrogen peroxide solution in drinking water resulted in mucosal hyperplasia of the duodenum

(small intestine) in male and female rats; no other effects were seen in the gastrointestinal tract or in other organs. Repeated inhalation exposures to hydrogen peroxide resulted in an inflammatory response in the larynx of male and female rats but not in any other locations of the respiratory tract, including the lung. In vitro genotoxicity tests have shown positive responses with hydrogen peroxide; however, in vivo studies are negative for genotoxicity. There are no adequate carcinogenicity, reproductive or developmental toxicity studies on hydrogen peroxide.

B. Acute Toxicity

The oral LD_{50} values of hydrogen peroxide (as 70% w/w aqueous solution) in rats are 1,026 mg/kg for males and 694 mg/kg for females (ECHA) [Kl. score = 1]. The oral LD_{50} values of hydrogen peroxide (as 35% w/w aqueous solution) in rats are 1,193 mg/kg for males and 1,270 mg/kg for females (EU 2003) [Kl. score = 1].

The 4-hour LC_{50} value of an aerosol of a 50% aqueous solution of hydrogen peroxide in rats is >170 mg/m^3 (EU 2015)[Kl. score = 1].

The acute dermal LD_{50} value of a 35% solution of hydrogen peroxide in rabbits is >2,000 mg/kg (EU 2003)[Kl. score = 1].

C. Irritation

Application of a 0.5 mL of a 10% aqueous solution of hydrogen peroxide to the skin of rabbits for 4 hours under semi-occlusive conditions was essentially non-irritating. The mean of the 24, 48, and 72 hour scores were: 0.08 for erythema and 0.00 for oedema (ECHA) [Kl. score = 1]. Application of 0.5 mL of a 35% aqueous solution of hydrogen peroxide to the skin of rabbits for 4 hours under semi-occlusive conditions was irritating. The mean of the 24, 48 and 72-hour scores were: 1.6 for erythema and 0.4 for oedema (EU 2003). [Kl. score = 1].

Instillation of 0.1 mL of a 3% aqueous solution of hydrogen peroxide into the eyes of rabbits was not irritating (ECHA) [Kl. score = 2]. Instillation of 0.1 mL of a 5% aqueous solution of hydrogen peroxide into the eyes of rabbits was slightly irritating. The mean of the 24, 48 and 72 hour scores were: 0.0 for corneal opacity; 0.00 for iridial lesions; 1.25 for conjunctival redness; and 0.00 for chemosis (ECHA) [Kl. score = 1]. Instillation of 0.1 mL of a 6% aqueous solution of hydrogen peroxide into the eyes of rabbits was irritating. There was slight to severe irritation in the unwashed or washed eyes of the tested animals, which were reversible in most animals within 72 hours following treatment. The treated eye in one animal was normal after 7 days. Moderate to severe corneal damage was seen in one rabbit (ECHA) [Kl. score = 2]. Instillation of 0.1 mL of a 10% aqueous solution of hydrogen peroxide into the eyes of rabbits was extremely irritating (EU 2003). [Kl. score = 1].

D. Sensitisation

Hydrogen peroxide (as a 3% aqueous solution) was not a skin sensitiser to guinea pigs in a Magnusson-Kligman test (EU, 2003). [Kl. score = 4]

E. Repeated Dose Toxicity

Oral

Male and female C57BL/6NCRIBR mice were given 35% aqueous solution of hydrogen peroxide in their drinking water for 90 days. Additional groups of animals were exposed for 90 days followed by a 6-week recovery period. The concentrations of hydrogen peroxide in the drinking water were 0, 100, 300, 1,000 or 3,000 ppm. The daily intakes were: 0, 26, 76, 239 and 547 mg/kg-day for males; and 0, 37, 103, 328 and 785 mg/kg-day for females. The strain of mouse was chosen because of their particular sensitivity to hydrogen peroxide due to a deficiency in the detoxification pathway of hydrogen peroxide. There were no deaths or clinical signs related to treatment. The 3,000 ppm males had significantly reduced body weights and body weight gain from Day 42 to the end of the exposure period. Feed and water consumption was significantly reduced in the 3,000 ppm animals, and in the 1,000 ppm females. At 300 ppm, there was a significant reduction of feed and water consumption on Day 35 of the study, but not at Day 63 or at the end of the exposure period. Total serum protein and serum globulin were significantly reduced in the 3,000 ppm males. Histopathological examination showed mild mucosal hyperplasia of the duodenum of the small intestine in 8/9 of the 3,000 ppm males and in 7/10 of the 1,000 ppm males. Minimal mucosal hyperplasia was also noted in 1/10 of the 300 ppm males. Minimal to mild mucosal hyperplasia was seen in 10/10 of the 3,000 ppm females and in 8/10 of the 1,000 ppm females. There were no other histopathologic effects in the gastrointestinal tract or in other organs. All effects were reversed following the 6-week recovery period. The NOAEL for systemic toxicity is 1,000 ppm in male mice (corresponding to 239 mg/kg-day). While feed and water consumption were significantly reduced in the 1,000 ppm females, there was no corresponding reduction in body weight or body weight gain (EU 2003). [Kl. score = 1]

Inhalation

Male and female Alpk:APfSD (Wistar-derived) rats were exposed by inhalation to 0, 2.03, 10.3 or 23.3 ppm 6 hours/day, 5 days/week for 28 days. Initially, the highest exposure group was 58.1 ppm; the exposure was reduced to 27.3 ppm and finally terminated because of the severity of toxicity of the exposure animals. Clinical signs were indicative of a respiratory tract irritant, and consisted of reddened noses, stains around the nose and abnormal respiratory noise. In general, the time of onset, the incidence and the severity of these clinical signs increased with exposure concentration and repeated exposure. The 23.3 ppm males had lower body weight gain and feed consumption. Serum albumin and total protein were significantly reduced in the 23.3 ppm animals. Histopathological changes were seen in the anterior-most regions of the nasal cavity lined with squamous epithelium of the $\geq$10.3 ppm animals; these changes were minimal to slight necrosis (with associated inflammation) and rhinitis. Inflammation and epithelial erosion in the larynx and increased perivascular neutrophil infiltration in the lungs were considered unlikely to be treatment-related because of an absence of a clear dose-response relationship. The NOEC for this study is 2.03 ppm or 2.9 mg/m^3 (EU 2003). [Kl. score = 1]

Dermal

No studies are available.

F. Genotoxicity

Per the results of the genotoxicity studies, hydrogen peroxide does not meet the current classification criteria for mutagenicity. Study details are provided below.

In Vitro Studies

A 3% aqueous solution of hydrogen peroxide was not mutagenic to *S. typhimurium* strains TA 1535, TA 1538, TA 1537 and TA 98 or *E. coli* strain WP2 with or without metabolic activation. It was mutagenic to *S. typhimurium* strain TA 100 with and without metabolic activation (Prival et al., 1991).

The *in vitro* cytogenetic studies of hydrogen peroxide were evaluated in the EU Risk Assessment Report (EU, 2003). Ten different studies were assessed which used different mammalian cell lines (CHO, CHL, CHC, V79, mouse skin cells and splenocytes, human embryonic fibroblasts, D98/AH2 [variant of HeLa] cells) and different endpoints (chromosomal aberration, micronucleus test, chromatid translocations). The studies without metabolic activation in total covered a concentration range from 0.83 μM to 7.35 mM. Only one study is available that evaluated the effect after metabolic activation with S9; the concentration range was 330 mM to 3.3 M. Eight of the 10 studies that tested without metabolic activation gave positive results. These data indicate that hydrogen peroxide has the potential to induce chromosomal aberrations in mammalian cells without metabolic activation.

The *in vitro* gene mutation studies in mammalian cells of hydrogen peroxide were evaluated in the EU Risk Assessment Report (EU, 2003). Eleven different studies were assessed which used different mammalian cell lines (CHO, V79 and others) and different endpoints (HGPRT, thymidine kinase, 6-thioguanine resistance, 6-azaguanidine resistance, ouabain resistance, mutation of the supF locus of the pZ189 plasmid). In total, the studies covered a concentration range from 0.2 μM to 10 mM. Positive results were seen in seven studies, negative results were seen in three studies, and one study gave ambiguous results (all without metabolic activation). In the only one study with metabolic activation, there was a negative result. These data indicate that hydrogen peroxide has the potential to induce mutations in mammalian cells without metabolic activation (EU, 2003)

In Vivo Studies

Male and female Swiss OF1 mice were given a single intraperitoneal injection of 0, 250, 500 or 1,000 mg/kg hydrogen peroxide. The polychromatic to normochromatic erythrocyte ratio (PCE/NCE) in bone marrow cells was significantly decreased, indicating cytotoxicity. There were no increases in the frequency of micronucleated erythrocytes in the bone marrow of treated animals at any dose level compared to the controls (EU 2003). [Kl. score = 1]

Male and female C57BL/6NCr1Br mice were given in their drinking water 0, 200, 1,000, 3,000 or 6,000 ppm hydrogen peroxide for 14 days. The daily intakes were: 0, 42.4, 164, 415 and 536 mg/kg-day for males; and 0, 48.5, 198, 485 and 774 mg/kg-day for females. There were no increases in the frequency of micronucleated erythrocytes in the bone marrow of treated animals at any dose level compared to the controls (EU 2003). [Kl. score = 1]

Male Wistar rats were administered intravenously 0, 25 or 50 mg/kg hydrogen peroxide. Animals were sacrificed either after 2-4 hours or 12-14 hours. The livers were removed; hepatocytes were

prepared in culture and then treated with [^{3}H]-thymidine. There was no induction of unscheduled DNA synthesis (UDS) in the hepatocytes from treated rats compared to the controls (EU 2003). [Kl. score = 2]

G. Carcinogenicity

No adequate studies are available.

H. Reproductive Toxicity

No adequate studies are available.

I. Developmental Toxicity

No adequate studies are available.

J. Derivation of Toxicological Reference And Drinking Water Guidance Values

NICNAS proposes a drinking water guideline (DWG) value of 1mg/L based on exposure to consumer products. However, in this application, as noted above, degradation of hydrogen peroxide is rapid and essentially complete once potentially released to the environment. Rather than apply the DWG value of 1 mg/L in the use of further risk assessment, the toxicological reference values developed for hydrogen peroxide follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011). Key in this application is the concept that under the use conditions employed in the field, hydrogen peroxide will degrade before consumer use would be expected and as such, the NICNAS DWG value is not relevant for this assessment.

Non-Cancer

Oral

A 90-day drinking water study was conducted on hydrogen peroxide using a strain of mouse that is sensitive to hydrogen peroxide because of a deficiency in the detoxication pathway (EU 2003). The NOAEL for systemic toxicity is 1,000 ppm in male mice (which corresponds to 239 mg/kg-day). At 3,000 ppm the male rats showed reduced body weights and body weight gain; reduced feed and water consumption; and serum chemistry changes. While reduced water and/or feed consumption were seen in the female mice at 1,000 and 3,000 ppm, there were no corresponding changes in the body weights or body weight gain. Mucosal hyperplasia of the duodenum (small intestine) was seen in the $\geq$1,000 ppm males and females. There were no other histopathologic effects in the gastrointestinal tract or in other organs. The NOAEL of 239 mg/kg-day will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10

UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 239/(10 x 10 x 1 x 3 x 1) = 239/300 = 1 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (1 x 70 x 0.1)/2 = 3.5 mg/L

Cancer

There are no adequate carcinogenicity studies on hydrogen peroxide. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Hydrogen peroxide does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Hydrogen peroxide is moderately toxic to aquatic organisms on an acute and chronic basis.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on hydrogen peroxide.

Table 3 Acute Aquatic Toxicity Studies on Hydrogen Peroxide

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hour LC_{50}	16.4	2	EU 2003
Daphnia pulex	48-hour LC_{50}	2.4	2	EU 2003
Daphnia magna	24-hour EC_{50}	3.3	2	EU 2003
Skeletonema costatum	72-hour EC_{50} NOEC	2.39 0.63	2	EU 2003

Chronic Studies

A NOEC from a 21-day *Daphnia sp* reproduction study on hydrogen peroxide was 0.63 mg/L (EU 2015). [Kl. score = 1]. The long-term NOEC value for *S. costatum* was 1.69 mg/L. (EU 2015) [Kl Score = 1].

C. Terrestrial Toxicity

No adequate studies are available.

D. Calculation of PNEC

The PNEC calculations for hydrogen peroxide follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (16.4 mg/L), invertebrates (2.4 mg/L) and algae (1.38 mg/L). Chronic toxicity studies are available for invertebrates (0.63 mg/L) and algae (0.63 mg/L). On the basis that the data consist of short-term results from three trophic levels and long-term results from two trophic levels, an assessment factor of 50 has been applied to the NOEC values of 0.63 mg/L for invertebrates and algae. The $PNEC_{water}$ is 0.013 mg/L.

PNEC sediment

No reliable experimental toxicity data on sediment organisms are available. The environmental distribution of hydrogen peroxide is dominated by its water solubility. The K_{oc} parameter does not readily apply to inorganics, such as hydrogen peroxide. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sediment}$. Based on its properties, no adsorption of hydrogen peroxide to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No reliable experimental toxicity data on terrestrial organisms are available. The environmental distribution of hydrogen peroxide is dominated by its water solubility. Sorption of hydrogen peroxide should be regarded as a reversible situation, *i.e.*, the substance is not tightly nor permanently bound. The K_{oc} parameter does not readily apply to inorganics, such as hydrogen peroxide. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{soil}$. Based on its properties,

hydrogen peroxide is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Hydrogen peroxide is normally a short-lived substance in the environment. It is biologically degraded by an enzyme-mediated process, which is rapid and can be considered equivalent to readily biodegradable. Abiotic degradation of hydrogen peroxide is also an important process. Thus, hydrogen peroxide does not meet the criteria for persistence.

Hydrogen peroxide is not expected to bioaccumulate because it is a reactive polar substance. Moreover, the estimated log K_{ow} is -1.57. Thus, it does not meet the screening criteria for bioaccumulation.

The NOEC values from chronic aquatic toxicity studies on hydrogen peroxide are >0.1 mg/L. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that hydrogen peroxide is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for hydrogen peroxide.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hydrogen Peroxide	7722-84-1	Not a PBT	No	No	No	No	No	No	2	3	2[a]

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

[a] – preponderance of data indicates appropriateness of Tier 2

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
CHC	combined hepatocellular cholangiocarcinoma cell
CHL	Chinese hamster lung cell
CHO	Chinese hamster ovary cell
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
HeLa	human cervix epitheloid carcinoma cell
HGPRT	hypoxanthine-guanine phosphoribosyltransferase
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
Kl	Klimisch scoring system
kPa	kilopascal
L	litre
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
M	molar
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mm	millimetre
mM	millimolar
mol%	gram molecular weight percent
mPa	millipascal

NCE	normochromatic erythrocyte
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
Pa*m^3 /mol	pascal meter cubed per mol
PBT	Persistent, Bioaccumulative and Toxic
PCE	polychromatic erythrocyte
PNEC	Predicted No Effect Concentration
ppm	parts per million
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
UDS	unscheduled DNA synthesis
V79	Chinese hamster lung, immortalized cell
w/w	weight/weight
wt%	weight percent
mM	micromolar

Qualitative Tier 2 Assessment

Hydrotreated Light Petroleum Distillate

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Hydrotreated light petroleum distillate is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Hydrotreated light petroleum distillate	64742-47-8	Surfactant	0.00099%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no carcinogenicity studies on hydrotreated light petroleum distillate, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Hydrotreated light petroleum distillate (CAS No. 64742-47-8)	Developmental Study	Reduced maternal body weight	500	1000	0.5	1.8

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Hydrotreated light petroleum distillate (CAS No. 64742-47-8)	*D. magna*.	0.48	100	0.005

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Hydrotreated light petroleum distillate (CAS No. 64742-47-8)	[a]	-	-	0.36

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Hydrotreated light petroleum distillate (CAS No. 64742-47-8)	[a]	-	-	0.32

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Hydrotreated light petroleum distillate is a complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

Hydrotreated light petroleum distillate is an Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB) substance containing aliphatic (linear, branched, and/or cyclic paraffins) molecules of carbon and hydrogen. The molecular structure for the UVCB substance was not available. The molecular structure for a representative substance in this group, hydrodesulfurized kersosine (CAS No. 64742-81-0), is presented in **Figure 1**.

Figure 1 Molecular Structure of Hydrosulfurized Kerosine[2]

Representative substances are expected to be readily biodegradable. They have a low potential to bioaccumulate. They are highly insoluble in water and have high adsorption potential. While sediment and soil are expected to be the main targets for environmental distribution, biodegradation potential is expected to offset sorption.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for hydrotreated light petroleum distillate is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

Hydrotreated light petroleum distillate exhibits low acute toxicity by the oral, inhalation and dermal routes. It is not irritating to the skin and eyes, but it is a skin sensitiser. Aside from minor changes in body weight, no adverse effects were seen in animals given repeated doses by the oral route. The substance is not genotoxic when tested in both in vitro and in vivo assays. There is no indication that this substance will cause malformations or have an adverse effect on reproduction and development. This information was derived in part from products of similar structure or composition.

In a developmental toxicity study, undiluted JP-8 jet fuel was administered to 30 Sprague-Dawley (Crl:CD) rats/dose by gavage at various volumes to achieve dose levels of 0 (sterile water), 500, 1000, 1500, or 2000 milligrams per kilogram body weight day (mg/kg bw/day) from days 6 through 15 of gestation. The no observed adverse effect level (NOAEL) for reduced maternal body weight is 500 milligrams per kilogram-day (mg/kg-day), based on reduced body weight in dams and in pups treated under a repeat dose regimen. NOAELs from repeated-dose toxicity studies were higher. Therefore, the NOAEL from the developmental toxicity study was used for determining the oral RfD and the drinking water guideline value (1.8 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Hydrotreated light petroleum distillates may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

[2] Source EPISUITE

There is low potential for human receptors to be exposed to hydrotreated light petroleum distillates in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, hydrotreated light petroleum distillates is readily biodegradable and does not persist in the environment.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, hydrotreated light petroleum distillates is a low toxicity concern to aquatic organisms. Acute toxicity towards fish, aquatic invertebrates and algae is of the same order of magnitude.

Hydrotreated light petroleum distillates is readily biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for hydrotreated light petroleum distillates are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNECs for water (see **Table 3**). There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method (see **Tables 4 and 5**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of hydrotreated light petroleum distillates in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, first, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The concentration of hydrotreated light petroleum distillates within the stimulation fluids will decrease in response to biodegradation and photolytic degradation of constituents over time. Chemical-specific biodegradation information presented in the dossier was used for the assessment.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

HYDROTREATED LIGHT PETROLEUM DISTILLATE

This dossier on hydrotreated light petroleum distillate presents the most critical studies pertinent to the risk assessment of this substance in its use in drilling muds and hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Hydrotreated light petroleum distillate was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. The substance was assessed as a tier 2 chemical for acute and chronic toxicity. Therefore, hydrotreated light petroleum distillate is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Hydrotreated light petroleum distillate is a complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

Representative substances are expected to be readily biodegradable. They are highly insoluble in water and have high adsorption potential. They have a low potential to bioaccumulate.

The substance has low acute toxicity by the oral and dermal route. It is not irritating to the skin and eyes, but it is a skin sensitiser. Aside from minor changes in body weight, no adverse effects were seen in animals given repeated doses by the oral route. The substance is not genotoxic when tested in both *in vitro* and *in vivo* assays. There is no indication that this substance will cause malformations or have an adverse effect on reproduction and development. The substance is of low acute concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 1,4-bis(propan-2-yl)benzene; 7,7-dimethylhexadecane; octadecane
CAS RN: 64742-47-8
Molecular formula: Not available (UVCB substance)
Molecular weight: Not available (UVCB substance)

Synonyms: Distillates, petroleum, hydrotreated light

3 PHYSICO-CHEMICAL PROPERTIES

Hydrotreated light petroleum distillate is a UVCB substance containing aliphatic (linear, branched, and/or cyclic paraffins) molecules of carbon and hydrogen. Physical and chemical properties were not available for the UVCB hydrocarbon. As a result, information was obtained from a read-across substance (hydrodesulfurized kerosine). Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Hydrodesulfurized Kerosine (CAS No. 64742-81-0)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	2	ECHA
Melting Point	-49°C (pour point) @ 101.3 kPa.	2	ECHA
Boiling Point[1]	90 to 320°C @ 101.3 kPa	2	ECHA
Density	770 to 850 kg/m^3 @ 15°C	2	ECHA
Vapour Pressure	<1,000 to 37,000 Pa at 37.8°C	2	ECHA
Partition Coefficient (log K_{ow})	1.99 – 18.02 @ 20°C	2	ECHA
Water Solubility	0.000009 – 0.00645 g/L @ 25 °C	-	OECD
Viscosity	1.1 to 2.5 mm^2/s @ 20°C (kinematic)	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for hydrotreated light petroleum distillates.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Representative substances are expected to be readily biodegradable. They are highly insoluble in water and have high adsorption potential. They have a low potential to bioaccumulate.

While sediment and soil are expected to be the main targets for environmental distribution, biodegradation potential is expected to offset sorption. In fact, fugacity modelling suggest that

[1] CAS numbers in this category indicate a boiling point range of 90-320 deg Celsius.

accumulation in sediment is expected to be several orders of magnitude less than 1%, relative to soil, water and air compartments.

B. Partitioning

Based on Henry's Law Constant values > 4.76 x 10^4 Pa-m^3/mol @25 °C, members of this group have the potential to volatilise from water or moist soil surfaces. These chemicals are unlikely to degrade by hydrolysis as they lack a functional group that is hydrolytically reactive. However, in the air, category members have the potential to rapidly degrade through indirect photolytic processes (OECD, 2012).

C. Biodegradation

Kerosines are readily to inherently biodegradable. In the supporting OECD 301 study, naphtha solvents were readily biodegraded in 28 days but not within the 10-day window. The mean of three samples was 61% theoretical biological oxygen demand on Day 28. In a valid OECD 301F supporting study Kerosine Mid-Blend was not considered readily biodegradable in 28 days, with less than 60% degradation on day 28 (58.6%). However, according to USEPA guidance for biodegradability, it is considered inherently biodegradable because significant degradation occurred). On the basis of this and the known properties of hydrocarbons in the range C9 to C16, kerosines are often considered not readily biodegradable; but as they can be degraded by microorganisms, they are regarded as being inherently biodegradable.

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

Standard adsorption/desorption studies are not applicable to petroleum UVCB substances. Mackay Level III modeling indicates that category member constituents partition mostly to the sediment and soil compartments rather than air compartment when an equal emission rate (1000 kg/hr) to the air, water, and soil compartment is assumed. When release occurs only to either the air, or soil compartment, constituents are indicated in the modeling to partition largely to the compartment to which they are released. When released to the water compartment, constituents are indicated by the model to partition to either water or sediment (HPVIS). However, based on the member category low solubility, partitioning to sediment would be expected.

E. Bioaccumulation

No experimental studies are available on the substance. Using BCFBAF in EPISuite™, the estimated BCF of a representative substance is 0.893 L/kg based on the Arnot-Gobas model that includes biotransformation and upper trophic. Thus, bioaccumulation is not expected (ECHA). [Kl. score = 2]

6 HUMAN HEALTH HAZARD ASSESSMENT

The information presented within this Section was derived in part from read-across substances: hydrodesulfurized kerosine (CAS No. 64742-81-0) and undiluted JP-8 jet fuel (CAS No. 8008-20-6).

A. Summary

The substance has low acute toxicity by the oral and dermal route. It is not irritating to the skin and eyes, but it is a skin sensitiser. Aside from minor changes in body weight, no adverse effects were seen in animals given repeated doses by the oral route. The substance is not genotoxic when tested in both *in vitro* and *in vivo* assays. There is no indication that this substance will cause malformations or have an adverse effect on reproduction and development. This information was derived in part from products of similar structure or composition.

B. Toxicokinetics

The studies of the pharmacokinetics (i.e. absorption, distribution, metabolism and excretion) of kerosine are scarce. There are some *in vitro* and *in vivo* studies available on jet fuels. However, because jet fuel is a complex mixture, these studies use certain constituents of jet fuels as marker compounds to describe the total jet fuel's pharmacokinetics. There are more data available for a number of kerosine constituents, and these can be used as a basis for understanding the pharmacokinetics of kerosine as a whole. There are three ways in which humans are exposed to kerosine: by inhalation; ingestion; and, dermal contact. Due to the relatively low volatility of kerosine and jet fuels, dermal exposure can be a more important route of exposure than exposure via inhalation. During many operations involving aircraft fuel tanks there is a significant potential for dermal exposure. Ingestion occurs primarily as a consequence of incidental ingestion.

Groups of five male C3H mice were dosed with a single dermal application of 15 or 60 µL kerosine (30% straight-run hydrotreated and 70% hydrocracked kerosine) spiked with radiolabeled naphthalene or tetradecane, and sacrificed after 96 h exposure (Mobil, 1994). Another group of five male C3H mice were exposed by air to the same compounds and doses in a metabolism cage to determine passive inhalation. The results of the dermal exposure show that 5% of the labelled tetradecane and 15% of the labelled naphthalene were absorbed over 96 h. The inhalation experiments showed that 2.8% of the labelled naphthalene was bioavailable. Comparison of these data with a similar dataset obtained with a 25% concentration of the test compounds diluted in mineral oil, revealed that dilution did not affect the absorption of the test compound.

Four groups of eight male Sprague-Dawley rats were exposed to 1, 4, 8,or 16 mL kerosine through the abdominal skin for 2 h at a skin area of 4, 8, 16 or 64 cm2, respectively (Tsujino et al., 2003). Before, during and after the experiment, blood samples were taken and analysed for trimethylbenzenes and aliphatic hydrocarbons. Trimethylbenzenes were detectable in blood within 5-20 min and showed a dose dependent absorption. High concentrations of aliphatic hydrocarbons were detected in the exposed skin as compared to the blood concentration. The aliphatic hydrocarbon levels were dependent on the amount of kerosine exposed per unit area.

The systemic distribution of kerosine components in the blood and tissues of rats following *in vitro* dermal exposures was investigated, using trimethylbenzenes and aliphatic hydrocarbons (C9-C16) as biomarkers (Tsujinoet al., 2002). The trimethylbenzenes were absorbed through the skin and detected in blood and tissues to a greater extent as compared to the aliphatics. The data indicate

that kerosine components are absorbed percutaneously and distributed to the various organs via the blood circulation. Distribution of trimethylbenzenes in blood and tissues following dermal exposure is (at decreasing concentrations): kidney > blood > liver > adipose > brain > spleen > lung = muscle. Distribution of aliphatics in blood and tissues following dermal exposure is (at decreasing concentrations): blood > adipose > muscle > lung > liver > kidney > spleen > brain.

The inhalation studies demonstrate that the volatile kerosine constituents are well absorbed (31 – 54%) and are distributed mainly in the fat tissue. Aromatics were metabolised at a higher rate than naphthenes, n-alkanes, isoalkanes and 1-alkenes. Dermal application of kerosine or jet fuel generally shows that the aromatics and aliphatics are well absorbed into the skin. Subsequently, the aromatics penetrate the skin at a higher rate than the alkanes. SKINPERM calculations indicate that although skin permeation rates of alkanes, naphthenes and aromatics are more or less comparable, the latency times of alkanes are longer than the latency times of naphthenes and aromatics. After absorption, the kerosine constituents are distributed via the blood circulation to the fat tissue and various organs. Studies with oral exposure to kerosine indicate that gastrointestinal absorption of kerosine is slow and incomplete, resulting in low bioavailability.

C. Acute Toxicity

Kerosines are of low acute toxicity, with an oral LD50 greater than 5000 mg/kg (rat), a dermal LD50 greater than 2000 mg/kg (rabbit), and an inhalation LC50 greater than 5.28 mg/L (rat). The most important effects in animals following very high oral doses were slight irritation of the stomach and the gastrointestinal tract. The only adverse effects observed in acute inhalation studies were decreased activity and breathing frequency at very high doses. Dermal application of kerosine did not lead to acute toxic systemic effects. Clinical effects observed were related to dermal irritation rather than to systemic toxicity. The acute toxicity of kerosine is not classified by EU CLP Regulation (EC No. 1272/2008).

Oral

In the key acute oral toxicity study (Klimisch score=1; ARCO, 1992a), groups of fasted (5 per sex), young adult, Sprague Dawley rats were given a single oral dose of undiluted thermocracked kerosine at a dose of 5000 mg/kg bw and observed for 14 days. There were no treatment related mortalities. All of the study animals exhibited one or more of the following clinical signs: nasal discharge, ocular discharge, abnormal stools, lethargy, stained coat, and alopecia. All animals gained weight during study period. At necropsy, one of the ten animals exhibited visual lesions, the remaining nine showed signs of alopecia in the inguinal and/or perineal regions. The oral LD50 was determined to be greater than 5000 mg/kg in males and females.

In supporting studies conducted on kerosine substances, rats were administered single oral gavage doses of the test substance. The results supported an oral LD50 of > 5000 mg/kg in males and females.

Inhalation

In the key acute inhalation toxicity study (Klimisch score = 1; API, 1987a), groups of Sprague-Dawley rats, five males and five females, were exposed by inhalation route to straight-run kerosine for 4 hours to their whole body at a single dose of 5.28 mg/L (vapour, analytical). All except one animal had normal growth rates throughout the study. The one exception on day 8 had a body weight less

than its starting body weight but by the end of the study normal growth had resumed. All animals exhibited decreased activity during the exposure. Otherwise there were no treatment-related clinical signs of toxicity. No macroscopic lesions were observed in any animal at post-mortem and no microscopic changes were observed in any lung section examined. The LC50 was greater than 5.28 mg/L.

In supporting studies conducted on kerosine substances, rats were administered single doses of the test substance via inhalation. The LC50s as measured based on mortality and systemic effects do not indicate classification of kerosine as an acute inhalation toxicant. One supporting study on deodorised kerosine showed a lack of systemic effects after repeated exposure to rats (6 hours each day for 4 days) and resulted in an LC50 of > 7.5 mg/L (Carpenter et al., 1976). Another supporting study on deodorised kerosine showed a lack of systemic effects after a single 6-hour exposure to cats, and resulted in an LC50 of > 6.4 mg/L (Carpenter et al., 1976).

Dermal

In the key acute dermal toxicity study (Klimisch score=1; ARCO, 1992g), groups of young adult New Zealand White rabbits, five males and five females, were dermally exposed to undiluted thermocracked kerosine for 24 hours to 10% of their body surface area at a dose of 2000 mg/kg. Animals were then observed for 14 days. There were no mortalities and all animals gained weight during the study. All of the animals exhibited one or more of the following clinical signs during the observation period: dermal irritation (erythema, edema, eschar, fissuring and/or dried skin) and/or abnormal stools. Apart from skin irritation, there were no other abnormalities noted at necropsy. The dermal LD50 was determined to be greater than 2000 mg/kg in both males and females.

In supporting studies conducted on kerosine substances, rabbits were administered single dermal doses of the test substance, and results supported a dermal LD50 of > 2000 mg/kg in males and females..

D. Irritation

Skin

In the key study, young adult rabbits (6 females) were dermally exposed (occlusive coverage) to 0.5 mL of undiluted kerosine/heating oil for 24 hours on both intact and abraded skin sites. Each of the test sites was evaluated for skin responses for 9 days post-exposure and was scored using the Draize scale. The mean erythema score from 24 to 72 hours was 3.46/4 while the mean edema score from 24 to 72 hours was 2.33/4. While this protocol deviates from current guidelines that state exposure should be semi-occlusive over 4 hours, and to intact skin only, this study is included as key to show the irritating nature of kerosine products.

In another guideline study conducted according to GLP and in accordance with current guidelines, young adult New Zealand White rabbits (3 per sex) were dermally exposed (semi-occlusive coverage) to 0.5 mL of undiluted odourless kerosine, for 4 hours. Animals were observed for seven days after exposure. Irritation was scored based on the Draize method (1959). The mean erythema score from 24 to 72 hours was 0.17/4 while the mean edema score from 24 to 72 hours was 0/4.

Additional supporting studies are provided on straight run kerosine, odourless kerosine, hydrocracked kerosine, hydrodesulfurised kerosine, Jet Fuel A, Jet Fuel A1, JP-5, and Cherry Point Jet

Fuel A. Most of the studies are valid in their methodology, but they differ from the current OECD guidelines in that animals were exposed under occluded conditions for 24 hours instead of semi-occluded conditions for 4 hours. Considering the conditions of the test, results must be interpreted carefully for the purposes of classification and labelling. The mean scores for erythema and edema have been assessed against the deviations, and provided the test would be conducted under standard conditions, the overall weight of evidence indicates that kerosines are irritating to skin. Kerosines are classified as irritating to the skin according to criteria in EU CLP Regulation (EC No. 1272/2008).

Effects on skin irritation/corrosion: irritating

Eyes

A number of well-controlled (GLP) animal experiments performed on a variety of kerosines indicate that none of the kerosines and jet fuels tested were more than slightly irritating to the eyes. In addition, a number of short reports on eye irritation studies on JP-5 and JP-8 show no eye irritation whatsoever in rabbits (6 unwashed eyes; 3 washed eyes): all scores 0.0 for up to 7 days (end of the study). None of the hazard assessments of kerosine and jet fuel constituents have resulted in classification for eye irritation.

In the key study selected for primary eye irritation, 0.1mL of undiluted thermocracked kerosine was instilled into the conjunctival sac of the right eye of three female young adult New Zealand White rabbits and observed through 72 hours. Irritation was scored according to the Draize method (1959). There was no evidence of damage to the cornea or iris for all animals over all scoring periods. Mild conjunctivae indicators such as redness, chemosis, and discharge were evident at the one-hour scoring interval, but not at any of the other scoring intervals. Fluorescein staining scores were zero for all study animals over all scoring periods.

The average irritation score was 0.0 for the cornea, iris and conjunctivae.

Based on the evidence, kerosine is not an eye irritant.

E. Sensitisation

In animal assays for skin sensitisation such as the Magnusson-Kligman GPMT and the Buehler assay, kerosines and jet fuels did not trigger a positive response.

In the key dermal sensitisation study (Klimisch score=1; ARCO, 1992q), thermocracked kerosine in mineral oil was tested on male young adult Pig/Hartley guinea pigs using a modified Buehler technique. During the challenge phase, a second exposure of a 1:4 dilution of thermocracked kerosine to induced test animals did not yield higher response grades, severity, or incidence than those associated with the naive challenge control group exposed to thermocracked kerosine. During the challenge phase, exposure of 0.2% DNCB to induction positive control animals elicited significantly higher response grades, severity indices, and incidence over the naive DNCB challenge control group. The vehicle irritation control group was free of dermal irritation during the challenge phase. Therefore, under the conditions of this study, thermocracked kerosine is not considered a delayed contact sensitiser while DNCB induced an appropriate positive response.

Based on test data, there was no evidence of skin sensitisation; therefore, kerosine is not classified for skin sensitisation according to EU CLP Regulation (EC No. 1272/2008)

F. Repeated Dose Toxicity

Oral

In the key oral subchronic study (Klimisch score=1; Mattie et al., 2000), male rats were treated for 70 to 90 days with 0 (1mL of distilled water), 750, 1500, or 3000 mg/kg/day of undiluted JP-8 jet fuel, then mated to untreated females (one female at a time). Males were gavaged throughout the cohabitation period and were returned to their individual cage after successful mating. In the second part of the study, female rats were administered the test compound at doses of 0 (1mL of distilled water), 375, 750, or 1500 mg/kg/day undiluted JP-8 jet fuel for 90-day prior to mating, through mating, gestation, delivery, and lactation for a total of 21 week. During mating, they were housed with untreated males.

There were no effects on clinical signs or mortality in either sex. Haematology, clinical chemistry, and urinalysis were measured only in females without any effects noted. Body weights in male rats were decreased in a dose-dependent manner and was likely related to nephropathy, which is specific in male rats treated with hydrocarbons, and not relevant for human exposure. In females, body weight was only significantly reduced in the high-dose group. Absolute and relative liver weights were increased in mid- and high-dose females, but were not likely biologically significant due to the lack of changes in clinical chemistry or histopathology in the liver. The test compound caused perianal dermatitis (high-dose only) and stomach hyperplasia (mid- and high-dose) in the female rats. There was a dose-related decrease in pup weight that was significant in the 750 mg/kg/day group on postnatal day 4 only and in the 1500 mg/kg/day group from postnatal day 4 through postnatal day 21 but had recovered by postnatal day 90. There were no treatment-related effects on reproduction or sperm parameters in males. There were no effects on reproduction, gestation, or litter size in females.

The study LOAEL for systemic effects is 1500 mg/kg/day and the NOAEL for systemic effects is 750 mg/kg/day, based on reduced body weight in dams and in pups. The LOAEL for adult males rats exposed to JP-8 orally was 750 mg/kg/day due to changes in clinical pathology, body weight, organ weights and the same irritation seen in female rats. The decrease in male rat bodyweight is very likely due to the male rat-specific nephropathy and is therefore not taken into account for the derivation of the oral NOAEL. The reproduction NOAEL was 3000 and 1500 mg/kg/day in males and females, respectively.

Inhalation

In a key subchronic inhalation toxicity study (Klimisch score=1; Mattie et al., 1991), JP-8 jet fuel was administered to 95 male Fisher 344 rats, 75 female Fischer 344 rats, and 100 male and female C57BL/6 mice by dynamic whole body vapour exposure at concentrations of 0, 500 or 1000 mg/m3(0, 0.5, or 1.0 mg/L) as a vapour for 24 hours per day, 7 days/week for a total of 90 days. The male rats developed hydrocarbon-induced nephropathy at both treatment concentrations. Male rats had decreased body weight and decreased absolute and relative kidney weight at both treatment concentrations. Female rats were unaffected by treatment. In mice, no significant clinical signs of toxicity were noted that differentiated the groups that were treatment-related. The NOAEC for male rats is difficult to establish, since potential adverse effects may be masked by male rat specific

hydrocarbon nephropathy. However, based on the hydrocarbon-induced nephropathy and reduced body weights and increased kidney weights, the LOAEC in male rats is 500 mg/m3. The LOEC for male mice is also 500 mg/m3, but it was not treatment related. The NOAEC for female rats and mice is greater than or equal to 1000 mg/m3. This was the highest dose tested in the study.

In a subacute inhalation toxicity study (Klimisch score = 1; API, 1986), hydrodesulfurised kerosine vapour was administered to 20 Sprague-Dawley rats/sex/concentration by dynamic whole body exposure at a concentration of 24 mg/m3(0.024 mg/L) for 6 hours per day, 5 days/week for 4 weeks. There were no compound related effects in mortality, clinical signs, body weight, haematology, clinical chemistry, organ weights, or gross and histologic pathology. Therefore, the NOAEC is greater than or equal to 24 mg/m3. This was the highest dose tested in the study.

Dermal

In a key sub-chronic dermal study hydrodesulfurized kerosine was applied at concentrations of 20, 40 or 60% (v/v) at a rate of 1 ml/kg/day to the shorn intrascapular region of groups of 12 individually housed male and female, Sprague-Dawley rats (aged 7-9 weeks). This was equivalent to doses of test material of 165, 330 or 495 mg/kg/day. Dosing was continued for five days a week for 13 weeks. In addition a group of 12 male and 12 female rats of similar age were administered mineral oil at a dose rate of 1 ml/kg/day; these animals served as vehicle controls. 12 rats/sex/group each in the vehicle controls and high dose group were maintained for a 4-week recovery period. Ingestion of the test material was prevented by using a collar and removal of any residual test or control material from the skin. Animals were observed for clinical signs prior to dosing and 1, 6 and 24 hours after the first dose. Subsequently, observations were made prior to each dose being applied.

Prior to the administration of each dose, the treated skin site was evaluated for dermal irritation using the Draize scoring method. Body weights were recorded prior to the first dose and weekly thereafter. An ophthalmic examination was conducted on each rat prior to application of the first dose and again prior to sacrifice at the end of the study. During the week prior to the first dose, each rat was subjected to a functional observation battery (FOB). The FOB was conducted again 1, 6 and 24 hours after the first dose and at 7 and 14 days. During the study, the FOB, motor activity and startle response testing was conducted on all rats at weeks 4, 8 and 12. At week 14 blood samples were collected from 12 animals/sex/group. Full necropsies were performed at week 14 on 6 rats/sex/group and at week 18 on the recovery rats (vehicle and high dose groups). Each full necropsy included an examination of the external surface of the body and its contents. The remaining six rats of each group were anesthetized with an intraperitoneal injection of Pentothal and transcardially perfused in-situ using 10% neutral-buffered formalin and given a limited necropsy. For these rats, no organs were weighed and specific tissues were also collected for subsequent microscopic testing.

There was a generally dose-related increase in the incidence and severity of various skin conditions at the treated site. Males seemed to be more sensitive than females as they were affected at all doses, however, the effects indicated very little irritation. Recovery group animals revealed complete recovery in the females and minimal hyperkeratosis in the high dose group males. At necropsy no substance-related observations were made for males in any group. In the females there was a suggestion of a possible treatment-related effect which occurred in 7 rats across all groups and consisted of skin crusts or ulceration at the site of application of test material. Haematological and serum clinical parameters were unaffected by treatment.

All animals survived until scheduled termination. There were no test substance-related effects on survival, clinical observations (apart from skin irritation), neurobehavioral signs or ophthalmological findings. The NOEL for systemic toxicity was >495 mg/kg/day. The LOEL for slight dermal irritation was 165 mg/kg/day, equivalent to ~ 1mg/cm2.

G. Genotoxicity

In vitro gene mutation in mammalian cells

Key in vitro gene mutation studies in mammalian cells were identified. In a study by the American Petroleum Institute (API, 1984b), cultures of mouse lymphoma cells were exposed to hydrodesulfurised kerosine with or without metabolic activation by Aroclor 1254-induced rat liver S9 fraction. Under non-activation conditions the test material induced a good range of toxicities for evaluation (relative growths ranged from 2.8% to 65.3%). None of the assays induced a mutant frequency that exceeded the minimum criterion (40.8 x 10-6). The test material was not mutagenic under non-activation conditions. In the presence of metabolic activation a wide range of toxicities was induced (6.1 to 107.9% relative growths). The minimum criterion mutant frequency of 69.0 x 10-6 was not exceeded. The test material was therefore considered non mutagenic under activation conditions. In a study by API (1977) (Klimisch score = 1), mouse lymphoma L5178Y cells were exposed to straight-run kerosine in acetone vehicle at concentrations ranging from 0.04 to 0.065 µL/mL (with metabolic activation) or 0.006 to 0.13 µL/mL (without activation). There was no evidence that straight-run kerosine induced mutant colonies over background levels.

In vitro cytogenicity in mammalian cells

Hydrodesulfurised kerosine was tested in the sister chromatid exchange assay using Chinese hamster ovary cells (API, 1988a). The assay was conducted with Aroclor-induced rat liver S-9 activation system. A small but statistically significant increase in the frequency of sister chromatid exchanges was observed at the high and low concentrations with metabolic activation. These increases appeared to be random and of no biological significance. There were no significant increases observed at any concentration in the absence of metabolic activation. Under the conditions of the study, hydrodesulfurised kerosine is considered to be negative in the sister chromatid exchange assay with Chinese hamster ovary cells.

In vivo cytogenicity

Based on weight of evidence kerosine substances were found to be non-mutagenic through cytogenic investigations.

In six in vivo bone marrow cytogenetic studies in the rat, there were no indications of chromosomal aberrations. Although an in vivo Sister Chromatid Exchange study in the mouse gave positive findings in the male group (but not in the females) the positive findings in the males were associated with signs of toxicity (lethargy and weight loss) at the very high top dose used in the study (4000mg/kg), both on the day of the administration of the kerosine and the day after (when they were sacrificed).

In a rat bone marrow micronucleus assay (API, 1985c, Klimisch score = 1), straight run kerosine (CAS# 800-20-6) was administered to Sprague Dawley rats. Straight run kerosine was not considered to induce chromosomal aberrations in bone marrow cells of rats. In another bone marrow

micronucleus assay (API, 1984b, Klimisch score = 1), hydrodesulfurised kerosine (CAS# 64742-81-0) was administered to rats. No clinical signs of toxicity were exhibited by the rats, and there was no significant increase in frequency of micronucleated polychromatic erythrocytes in bone marrow as compared to control. In a study by API (1977) (Klimisch score = 1), straight-run kerosine (CAS# 8008-20-6) was administered to 45 male rats. No significant increase in the frequency of micronucleated polychromatic erythrocytes was observed.

In vivo gene mutation

Key in vivo gene mutation studies were identified. In a sperm cell dominant lethal mutation assay (API, 1980b, Klimisch score = 1), Jet Fuel A was administered via inhalation route to male mice at concentrations of 100 or 400 ppm for a 6-hour exposure period, 5 days per week for 8 weeks. Males were mated with females, and the uteri of pregnant females were examined for living and dead implants. Jet Fuel A did not increase the incidence of post-implantation deaths. In another study by API (1973) (Klimisch score = 1), deodorised kerosine was administered subcutaneously to 10 male Swiss-Webster mice in corn oil vehicle or intraperitoneally to 10 Long-Evans rats undiluted at a dose of 1.0 mL/kg. Males were mated with females, and no pattern of decreased pregnancy rate or increased embryo loss was observed in the females.

H. Carcinogenicity

Kerosine is not carcinogenic when animals are exposed via the oral or inhalation route (ECHA).

Male mice were administered dermally 37.5µL of jet fuel A to the shaved backs of 50 mice per dose, twice a week for 2 years or intermittently so that application of the jet fuel was suspended when dermal irritation was noted in 20% of the group and was resumed when irritation resolved in all but 20% of the affected animals. There was a significant increase in tumours at the application site with continuous treatment compared to the control (0% versus 44%), but not with intermittent treatment (0% versus 2%). With continuous treatment, there was a treatment-related increase in dermal tumour incidence compared to controls. However, stopping treatment during dermal irritation nearly eliminated the carcinogenic effect (ECHA) [Kl. Score = 1].

Male and female mice were administered dermally 25 mg of petroleum-derived jet fuel A to the shaved backs of 25 mice, three times a week for 105 weeks. Due to high mortality, jet fuel A application was discontinued during week 62, but surviving animals were observed until study termination. There was a significant increase in tumours at the application site (0%, 26%, and 26% in the controls, JP-4, and jet A groups). The majority of the tumours were squamous cell carcinomas or fibrosarcomas. At the doses tested, there was a treatment-related increase in dermal tumour incidence when compared to controls. The results of the study indicate that there was a treatment-related increase in dermal tumour incidence when compared to controls, therefore it can be concluded that Jet fuel A has a carcinogenic effect on mice at 25 mg dosage (ECHA) [Kl. Score = 1].

Straight-run kerosine (CAS # 8008-20-6) and hydrodesulfurised kerosine (CAS # 64742-81-0) were tested in standard 2-year bioassays in mice. The animals, 50 per group, were treated twice weekly with 50 µl straight-run kerosine or with hydrodesulfurised kerosine. It was concluded that both straight-run and hydrodesulfurised kerosine were moderate skin carcinogens (ECHA) [Kl. Score = 2].

In the key carcinogenicity study from NTP, JP-5 navy fuel in acetone was administered to 50 mice dermally at dose levels of 0 (vehicle control), 250, or 500 mg/kg bw/day for up to 103 weeks. There

was a significant decrease in survival in females at both treatment doses. Remaining high-dose females were sacrificed at week 90. There was no treatment-related effect on survival in male mice. The LOAEL is 250 mg/kg/day, based on dermatitis and decreased survival in females. No NOAEL can be determined. At the doses tested, there was not a treatment-related increase in tumour incidence when compared to controls (ECHA) [Kl. Score = 1].

The potential influence of skin irritation on tumour development in long-term mouse skin painting studies was investigated as part of the CONCAWE middle distillates programme. The study included straight run hydrotreated kerosine (MD3). The test material was applied to the shorn skin of three groups of 50 male mice for 104 weeks. For the straight run hydrotreated kerosine, skin tumours only developed in the group of animals in which substantial skin irritation occurred during the study. Since no polycyclic aromatic compounds were detected in the straight run kerosine it is concluded that the occurrence of tumours is likely to have been caused by a non-genotoxic mechanism. This conclusion is consistent with reports by others that lighter middle distillates are tumour promotors but not initiators and furthermore that skin irritation plays an important role in skin tumour development. These tumours are probably the consequence of a continuous cycle of cell damage and repair caused by chronic skin irritation. The conclusions gained from this study can be applied to other carcinogenicity studies on kerosines, and they show that tumours are noted in the presence of repeated dermal irritation, and that kerosines lack a genotoxic mechanism of carcinogenicity (ECHA) [Kl. Score = 1].

I. Reproductive Toxicity

There are no specific reproductive toxicity data for the substance but there are data available with ECHA as migrated information which is read-across based on grouping of substances (category approach).

An OECD Guideline 415 One-Generation Reproduction Toxicity study was conducted. This was a reproductive study performed in two parts. In the first part, males were treated for 70 to 90 days with 0 (1mL of distilled water), 750, 1500, or 3000 mg/kg/day of undiluted JP-8 jet fuel, then mated to untreated females (one female at a time). In the second part of the study, female rats were administered the test compound at doses of 0 (1mL of distilled water), 375, 750, or 1500 mg/kg/day undiluted JP-8 jet fuel for 90 -day prior to mating, through mating, gestation, delivery, and lactation for a total of 21 weeks.

There were no changes in clinical signs or mortality in parental animals. Body weights in male rats were decreased in a dose-dependent manner. Terminal body weights were approximately 545 grams, 520 grams, 475 grams, and 315 grams in the control, 750, 1500, and 3000 mg/kg/day, respectively. In females, body weight was only significantly reduced in the high-dose group, but the differences were not significant at terminal sacrifice. The body weight in females at 20 weeks (1 week before sacrifice) was approximately 400 grams, 385 grams, 382 grams, and 335 grams in the control, 375, 750, and 1500 mg/kg/day, respectively. Hematology was not measured in the males and no effects were noted in the females. Clinical chemistry was not measured in the males and no effects were noted in the females. Urinalysis was not measured in the males and no effects were noted in the females. Absolute and relative liver weights were increased in mid- and high-dose females, but were not accompanied by any histological findings. The test compound caused perianal dermatitis (high-dose only) and stomach hyperplasia (mid- and high-dose) in the female rats.

There were no treatment-related effects on reproduction or sperm parameters in males. There were no effects on reproduction, gestation, or litter size in females. The lowest NOAEL based on parental body weight was determined to be 750 mg/kg/day.

The F1 generation was not examined for clinical signs though no mention would suggest no significant signs were noted. No mortality was observed. There were no effects on offspring viability. However, there was a dose-related decrease in pup weight that was significant in the 750 mg/kg/day group on postnatal day 4 only and in the 1500 mg/kg/day group from postnatal day 4 through postnatal day 21. The 1500 mg/kg/day group recovered by postnatal day 90. The NOAEL based on offspring body weight was determined to be 750 mg/kg/day.

J. Reproductive Toxicity/Developmental Toxicity

In a developmental toxicity study, undiluted JP-8 jet fuel was administered to 30 Sprague-Dawley (Crl:CD) rats/dose by gavage at various volumes to achieve dose levels of 0 (sterile water), 500, 1000, 1500, or 2000 mg/kg bw/day from days 6 through 15 of gestation.

There was a significant decrease in maternal weight gain with doses of 1000 mg/kg/day or greater. Maternal necropsy weight was significantly different than the control in the 1500 and 2000 mg/kg/day groups. There were no apparent clinical signs of toxicity. Reproductive endpoints were not assessed in this study because females were pregnant prior to treatment and did not deliver, so only developmental endpoints can be assessed. Thirteen females (one 1000 mg/kg/day; three 1500 mg/kg/day, and nine 2000 mg/kg/day) were found dead. Although there appears to be a dose-dependent increase in the mortality, necropsy found the cause of death to be related to the presence of the test compound in the lungs indicating dosing into the lungs instead of the gastrointestinal tract. The maternal LOAEL is 1000 mg/kg/day, based on reduced body weight gain. The maternal NOAEL is 500 mg/kg/day.

There was a significant decrease in fetal weight in both male and female fetuses dosed with 1500 and 2000 mg/kg/day. The test compound did not significantly increase the incidence of malformations or variations compared to the control nor was the sex ratio altered. The developmental LOAEL is 1500 mg/kg/day, based on reduced fetal weight. The developmental NOAEL is 1000 mg/kg/day. It can be concluded that the test substance is not toxic to development.

This study received a Klimisch score of 1 and is classified as reliable without restrictions because it was carried out in a method equivalent/similar to OECD TG 414.

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for the substance follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

<u>Non-Cancer</u>

The NOAEL for reduced maternal body weight is 500 mg/kg/day, based on reduced body weight in dams and in pups treated under a repeat dose regimen. The NOAEL from this study will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 500 /(10 x 10 x 1 x 10 x 1) = 500/1,000 = 0.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.500 x 70 x 0.1)/2 = 1.8 mg/L

Cancer

There are no carcinogenicity studies on the substance or related hydrocarbons. Thus, a cancer reference value was not derived.

L. HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

The substance does not exhibit the following physico-chemical properties:

- Explosivity
- Oxidizing potential

The substance is classified as a “Flammable Liquid Category 3”

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The substance is of low acute concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on hydrotreated light petroleum distillate surrogates.

Table 3 Acute Aquatic Toxicity Studies on Hydrotreated Light Petroleum Distillate Surrogate[2]

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hour LL_{50}	2-5	1	ECHA
Daphnia magna	48-hour EL_{50}	1.4	1	ECHA
Raphidocelis subcapitata	72-hour EC_{50}	<1-3 (average of 2)	1	ECHA
Selenastrum capricornutum	72-hour EC_{50}	3.7	2	ECHA

Chronic Studies

There are no long-term toxicity studies on fish. A single long term study on invertebrates is discussed below.

In a 21-day semi-static chronic reproductive toxicity test (OECD 211; KS = 1) on *Daphnia magna*, hydrodesulfurised kerosine was evaluated using water accommodated fraction methodology. The actual loading rates were 0 (control), 0.08, 0.19, 0.48, 1.2 and 3.0 mg/L. Under the conditions of this test, the 21-day chronic reproductive NOEL for kerosine is 0.48 mg/L. The LOEL is 1.2 mg/L. The EL_{50} based on reproduction is 0.89 mg/L (ECHA).

C. Terrestrial Toxicity

There are no terrestrial toxicity studies for this substance.

[2] Hydrodesulfurized Kerosine (CAS No. 64742-81-0)

D. Calculation of PNEC

The PNEC calculations for hydrotreated light petroleum distillate follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available from acute tests on three trophic levels. There is one long term study on a single trophic level organism, *D. magna*.

On the basis that the data consists of short-term studies from three trophic levels and a long-term study from one trophic level, an assessment factor of 100 is applied to the 21-day chronic reproductive NOEL for kerosine of 0.48 mg/L. The $PNEC_{aquatic}$ is 0.005 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.36 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (93.4/1280) \times 1000 \times 0.005$
$= 0.36$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3) [calculated]
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 193/1000 \times 2400]$
$= 93.4\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg).[calculated]
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 4818 \times 0.04$
$= 193$ L/kg

Where:
K_{oc} = organic carbon normalized distribution coefficient (L/kg). The K_{oc} for hydrodesulfurized kerosine calculated from EPISUITE™ using the MCI is 4818 L/kg.
F_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no experimental toxicity testing results available for the substance or its noted surrogates. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.32 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (96.4/1500) \times 1000 \times 0.005$
$= 0.32$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m3/m3)
BD_{soil} = bulk density of soil (kg/m3) = 1,500 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 4818 \times 0.02$
$= 96.4\ m^3/m^3$

And:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for hydrodesulfurized kerosine calculated from EPISUITE™ using the MCI is 4818 L/kg.
F_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

The substance or similar compounds are readily biodegradable; thus they do not meet the screening criteria for persistence.

Based on the estimated BCF values, derived from EPISuite estimates (BCF = 3.162 L/kg wet-weight) the substance does not meet the screening criteria for bioaccumulation.

The NOEC values from acute and chronic aquatic toxicity studies on the substance indicate it does not meet the screening criteria for toxicity.

Therefore, hydrotreated light petroleum distillates are not PBT substances.

B. Other Characteristics of Concern

No other characteristics of concern were identified for hydrotreated light petroleum distillates.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hydrotreated Light Petroleum Distillates	64742-47-8	Not a PBT	No	No	No	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
°F	degrees Fahrenheit
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	bioconcentration factor/bioaccumulation factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EL	effect level
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
KOWWIN	USEPA modelling program to estimate the organic carbon-normalised sorption coefficient for soil and sediment
kPa	kilopascal
L/kg	litres per kilogram
LL	Lethal loading
MCI	molecular connectivity index
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal

Pa.s64742	pascal second
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
					0	30	0	30	0	30	
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	64742-47-8	9.90E+00	1.50E+02	1.32E+00	1.32E-01	1.15E-01	1.32E-03	1.15E-03	2.64E-05	2.30E-05	5.00E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Qualitative Tier 2 Assessment

Isotridecanol, ethoxylated

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Isotridecanol, ethoxylated is a chemical in a product used in drilling and completion activities, including workovers. The workover process is designed to remove any solids from the well and facilitate placement of the pump. As part of this process, fluids and some coal fines are removed from the well and transported to produced water ponds for management within the produced water stream. Once the well has been placed and commissioned, produced water is discharged into the water gathering pipelines and conveyed to the water ponds/water treatment facilities, such as ROP2, for treatment and beneficial use (such as dust suppression, construction, operational use and stock water for cattle).

The purpose and maximum quantity for this chemical is summarized in **Table 1**.

Table 1 Initial and Underbalance Workover Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Isotridecanol, ethoxylated-	69011-36-5	Activators, Emulsifiers and Neutralisers	NA

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number
NA = quantity used varies

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on isotridecanol, ethoxylated. The alcohol ethoxylates $C_{12\text{-}13}AE_{6.5}$ and $C_{14\text{-}15}AE_{7}$ were not carcinogenic to rats in a two-year dietary study. Thus, a cancer reference value was not derived and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Isotridecanol, ethoxylated (69011-36-5)	2-year dietary study in rats	Increased organ weight	50	100	0.5	1.8

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Isotridecanol, ethoxylated (69011-36-5)	-	-	-	0.140[a]

[a] $PNEC_{water}$ for isotridecanol, ethoxylated is the ANZG Water Quality Guideline – Freshwater Trigger Value for Alcohol Ethoxylates (AE).
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Isotridecanol, ethoxylated (69011-36-5)	[a]	-	-	0.71

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Isotridecanol, ethoxylated (69011-36-5)	[a]	-	-	0.56

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this TIer 2 chemical is provided in the following sections.

General Overview

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x-y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerisation is indicated by the subscript (n) which indicates the average number of ethylene oxide units. Isotridecanol, ethoxylated has an average number of 1 to 2.5 moles of ethylene oxide (EO) units.

Isotridecanol, ethoxylated is a substance of unknown or variable composition, complex reaction products or biological materials (UVCB). A representative molecular structure of an AE is presented in **Figure 1**.

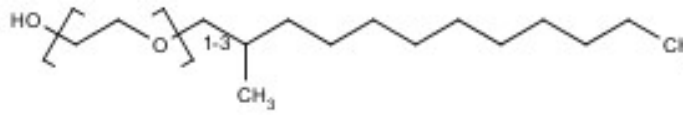

Figure 1 Representative Molecular Structure of Isotridecanol, ethoxylated[2]

Isotridecanol, ethoxylated is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for absorption to soil and sediment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for isotridecanol, ethoxylated is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the chemical is not a PBT substance.

Human Health Hazards

The acute toxicity of isotridecanol, ethoxylates is low by the oral and dermal routes. The skin irritation rabbit studies on isotridecanol, ethoxylated and similar alcohol ethoxylates show that the degree of irritation depends on the testing conditions and length of the exposure period. Human patch studies on these alcohol ethoxylates do not support a skin irritant classification. Isotridecanol, ethoxylated with EO units of 1 to <2.5 are not irritating to the eyes of rabbits. Isotridecanol, ethoxylated is not a skin sensitiser.

Repeated dose toxicity studies on alcohol ethoxylates similar to isotridecanol, ethoxylates in rats do not indicate any target organ effects. These alcohol ethoxylates are not genotoxic or carcinogenic and have a low potential for reproductive and developmental toxicity.

A two-year dietary study in rats has been conducted on a similar alcohol ethoxylate ($C_{12\text{-}13}AE_{6.5}$) (HERA, 2009). The no observed adverse effects level (NOAEL) from this study is 50 milligrams per kilogram-day (mg/kg-day) based on increased organ weights. The NOAEL was used to derive the oral RfD and the drinking water guidance value (1.8 milligrams per litre [mg/L]) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Isotridecanol, ethoxylates may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to isotridecanol, ethoxylates in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies

[2] Source https://echa.europa.eu/brief-profile/-/briefprofile/100.105.729

of the reverse osmosis system. In addition, isotridecanol, ethoxylates is expected to be readily biodegradable in the environment. In an OECD 301B test, degradation was 75% in 28 days (ECHA).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, isotridecanol, ethoxylated is of moderate toxicity concern to aquatic organisms. Acute toxicity towards fish, aquatic invertebrates and algae is of the same order of magnitude (ECHA).

Isotridecanol, ethoxylated is biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for isotridecanol, ethoxylated are provided in **Tables 3-5**. Isotridecanol, ethoxylated is an alcohol ethoxylate (AE). ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 0.14 mg/L for AE. This value was derived using data normalised to an alkyl chain length of C13.3 and EO of 8.2 using the statistical distribution method with 95% protection.

There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware

of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, estimated Water Management Facility (WMF) pond influent concentrations (2.2×10^{-7} mg/L, refer **Attachment 2**) are well less than PNECs for aquatic receptors (1.4×10^{-1} mg/L). Blending within the storage pond, degradation during storage and treatment would further reduce concentrations.

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Attachment 1 Risk Assessment Dossier

ETHOXYLATED BRANCHED C13 ALCOHOL
[ISOTRIDECANOL, ETHOXYLATED]

This dossier on isotridecanol, ethoxylated presents the most critical studies pertinent to the risk assessment of isotridecanol, ethoxylated in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products: Alcohol Ethoxylates (HERA, 2009). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Isotridecanol, ethoxylated was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Isotridecanol, ethoxylated was assessed as a tier 2 chemical for acute and chronic toxicity. Therefore, this substance is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Alcohol ethoxylates (AE) are a very widely used class of non-ionic surfactants. Significant quantities of AE are converted to alcohol ethoxysulphates (AES) with the remaining AE used primarily in household laundry detergents. AE have many desirable characteristics such as rapid biodegradation, low to moderate foaming ability, superior cleaning of man-made fibres and tolerance of water hardness. AE are also used in lesser quantities in household cleaners, institutional and industrial cleaners, cosmetics, agriculture and in textile, paper, oil and other process industries.

Isotridecanol, ethoxylated is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for adsorption to soil and sediment.

The acute toxicity of isotridecanol, ethoxylates is low by the oral and dermal routes. The skin irritation rabbit studies on isotridecanol, ethoxylated and similar alcohol ethoxylates show that the degree of irritation depends on the testing conditions and length of the exposure period. Human patch studies on these alcohol ethoxylates do not support a skin irritant classification. Isotridecanol, ethoxylated with EO units of 1 to <2.5 are not irritating to the eyes of rabbits. Isotridecanol, ethoxylated is not a skin sensitiser. Repeated dose toxicity studies on alcohol ethoxylates similar to isotridecanol, ethoxylates in rats do not indicate any target organ effects. These alcohol ethoxylates are not genotoxic, carcinogenic and have a low potential for reproductive and developmental toxicity. Isotridecanol, ethoxylated has moderate chronic toxicity concern to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Isotridecanol, ethoxylated
CAS RN: 69011-36-5
Molecular formula: Not available (UVCB substance)
Molecular weight: Not available (UVCB substance)

Synonyms: Isotridecanol, ethoxylated; C13 ethoxylated alcohol; Alcohol C13 ethoxylated; ethoxylated branched C13 alcohol

3 PHYSICO-CHEMICAL PROPERTIES

Alcohol ethoxylates (AE) are a class of non-ionic surfactants that have the basic structure $C_{x-y}AE_n$. The subscript (x-y) following the 'C' indicates the range of carbon chain units. The hydrocarbon chain can be either linear or branched. AEs also contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerisation is indicated by the subscript (n) which indicates the average number of ethylene oxide units. Isotridecanol, ethoxylated (CAS No. 69011-36-5) has an average number of 1 to 2.5 moles of ethylene oxide units.

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Isotridecanol, ethoxylated (1 to 2.5 moles ethoxylated)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear liquid with a rancid odour	2	ECHA
Melting Point	-11.6°C @ 101.3 kPa	1	ECHA
Boiling Point	>280°C @ 101.3 kPa	1	ECHA
Density	907 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	<5 Pa @ 20°C	2	ECHA
Partition coefficient (log K_{ow})	4.9* (calculated) @25 °C	2	ECHA
Water Solubility	0.02-0.029 g/L @ 21°C	1	ECHA
Dissociation Constant (pKa)	Not applicable	-	ECHA
Viscosity	38.2 mm^2/s (static) @ 20°C	1	ECHA

*Weight-averaged log K_{oc} of whole substance based on normalised composition.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No other specific environmental regulatory controls or concerns were identified within Australia and internationally for isotridecanol, ethoxylated.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Isotridecanol, ethoxylated is readily biodegradable. It has a low potential for bioaccumulation and a moderate potential for adsorption to soil and sediment.

B. Partitioning

Abiotic degradation like hydrolysis and photolysis is not an important process in case of alcohol ethoxylates due to the chemical structure of these substances (ECHA).

C. Biodegradation

Isotridecanol, ethoxylated is readily biodegradable. In an OECD 301B test, degradation was 75% in 28 days (ECHA) [Kl. score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

Using KOCWIN v2.00, the following calculated K_{oc} values were obtained: 441.7 for alcohol, C13, branched; 359.3 for alcohol ethoxylate, C13, branched, 1 EO; and 237.8 for alcohol ethoxylate, C13, branched, 3 EO (ECHA) [Kl. Score = 2]. The average of the K_{oc} values for the C13 ethoxylated alcohols, which is 298.6 L/kg, will be used to calculate the PNEC values for sediment and soil.

If released to soil, the average K_{oc} values for the C13 ethoxylated alcohols indicate a moderate potential for both adsorption and mobility. If released to water, based on these K_{oc} values and slight solubility, this substance may have moderate adsorption to suspended solids or sediment.

E. Bioaccumulation

The BCF values for alcohol ethoxylates in fathead minnows have been reported to range from <5 to 387.5 (Toll et al., 2000). The uptake rates varied from 330 to 1660 (L x kg/d) and elimination rates varied from 3.3 to 59 per day (Toll et al., 2000). The high concentrations in fish are thought to be prevented by an efficient biotransformation of the alcohol ethoxylates, leading to a high elimination rate. Thus, it can be stated that bioaccumulation of alcohol ethoxylates is regarded to be negligible as the surfactants will be rapidly metabolised (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of isotridecanol, ethoxylates is low by the oral and dermal routes. The skin irritation rabbit studies on isotridecanol, ethoxylated and similar alcohol ethoxylates show that the degree of irritation depends on the testing conditions and length of the exposure period. Human patch studies on these alcohol ethoxylates do not support a skin irritant classification. Isotridecanol, ethoxylated with EO units of 1 to <2.5 are not irritating to the eyes of rabbits. Isotridecanol,

ethoxylated is not a skin sensitiser. Repeated dose toxicity studies on alcohol ethoxylates similar to isotridecanol, ethoxylates in rats do not indicate any target organ effects. These alcohol ethoxylates are not genotoxic, carcinogenic and have a low potential for reproductive and developmental toxicity.

B. Acute Toxicity

The oral LD_{50} in rats for $C_{12\text{-}13}AE_{6.5}$ is 2,100 mg/kg (HERA, 2009) [Kl. score = 2]. The oral LD_{50} in rats for $C_{12\text{-}15}AE_7$ is 1,700 mg/kg (HERA, 2009) [Kl. score = 2].

An OECD Guideline 403 (Acute Inhalation Toxicity) study was conducted using Sprague Dawley rats exposed to 1600 mg/m^3 over a four hour period. The LC_{50} for this test was determined to be > 1 600 mg/m^3 (ECHA)[Kl Score = 2].

An acute dermal LD_{50} values of >2,000 mg/kg were determined for $C_{12\text{-}14}AE_3$ and $C_{12\text{-}14}AE_6$ in two separate studies (HERA, 2009) [Kl. score = 2]. The acute dermal LD_{50} of $C_{12\text{-}15}AE_7$ is >2,000 mg/kg (HERA, 2009) [Kl. score = 2].

C. Irritation

<u>Skin</u>

Application of 0.5 mL isotridecanol, ethoxylated (3 EO) to the skin of rabbits for 4 hours under occlusive conditions was considered irritating (ECHA) [Kl. score = 2].

Application of 0.5 mL isotridecanol, branched, ethoxylated (3-4 EO) to the skin of rabbits for 24 hours under occlusive conditions was considered irritating (ECHA) [Kl. score = 2].

Application of 0.5 mL isotridecanol, ethoxylated (3 EO) to the skin of rabbits for 4 hours under semi-occlusive conditions was not considered irritating (ECHA) [Kl. score = 2].

Application of 0.5 mL $C_{12\text{-}13}AE_{<2.5}$ (CAS No. 66455-14-9) to the skin of rabbits for 24 hours under occlusive conditions was considered irritating (ECHA) [Kl. score = 2].

Application of 0.5 mL alcohols C12-13, branched and linear, <2.5 EO to the skin of rabbits for 4 hours under occlusive conditions was not considered irritating (ECHA) [Kl. score = 2].

In a 24-hour human patch test, there was some short-lived redness in some individuals from the application of $C_{12\text{-}14}AE_3$, but there was no scaling or oedema in any subjects (HERA, 2009) [Kl. score = 2].

In a standard 4-hour human patch test, the irritation potential of $C_{12\text{-}15}AE_5$ and $C_{12\text{-}15}AE_5$ were compared to 20% sodium dodecyl sulfate (which is classified a skin irritant under GHS). The results showed that neither alcohol ethoxylate should be classified as a skin irritant (Basketter et al., 2004) [Kl. score = 2].

Eye

Instillation of 0.1 mL isotridecanol, ethoxylated (3 EO) (CAS No. 69011-36-5) into the eyes of rabbits was severely irritating. The means of the 24, 48 and 72-hour scores were: 1.6 for corneal opacity; 0.6 for iridial lesions; 2.2 for conjunctival redness; and 0.7 for chemosis. The effects were not fully reversible within 21 days (ECHA) [Kl. score = 2].

Instillation of 0.1 mL isotridecanol, branched, ethoxylated (3-4 EO) (CAS No. 24938-91-8) into the eyes of rabbits was severely irritating. The means of the 24, 48, and 72-hour scores were: 1.0 for corneal opacity; 0.1 for iridial lesions; 1.7 for conjunctival redness; and 0.6 for chemosis. The effects were not fully reversible within 8 days (ECHA) [Kl. score = 2].

Instillation of 0.1 mL alcohols C12-13, branched and linear, <2.5 EO (CAS No. 160901-19-9) into the eyes of rabbits was not irritating. The means of the 24, 48, and 72-hour scores were: 0.00 for corneal opacity; 0.00 for iridial lesions; 0.83 for conjunctival redness; and 0.50 for chemosis (ECHA) [Kl. score = 2].

Instillation of 0.1 mL $C_{12\text{-}13}AE_{<2.5}$ (CAS No. 66455-14-9) into the eyes of rabbits was not irritating. The mean of the 24, 48, and 72-hour scores were: 0.00 for all endpoints (ECHA) [Kl. score = 2].

D. Sensitisation

No sensitisation studies are available on isotridecanol, ethoxylated.

In a guinea pig maximisation test, $C_{12\text{-}13}AE_{<2.5}$ (CAS No. 66455-14-9) was not considered a skin sensitiser (ECHA) [Kl. score = 2].

E. Repeated Dose Toxicity

Oral

No repeated dose toxicity studies are available on isotridecanol, ethoxylated.

Rats were given in their diet 0%, 0.0313%, 0.0625%, 0.125%, 0.25%, 0.5% or 1.0% $C_{12\text{-}15}AE_7$ for 90 days. The animals in the $\geq$0.25% groups showed significantly reduced body weight gain, which was associated with marked decreases in food and water consumption. Relative liver weights were significantly increased in the $\geq$0.5% male rats and $\geq$0.25% females. Histopathologic examination showed hepatocytic enlargement in the $\geq$0.125% groups, suggesting increased liver metabolism on the basis of increased alkaline phosphatase activity at the higher dose levels. The NOAEL was established at 0.0625% in the diet or 102 mg/kg-day (HERA, 2009) [Kl. score = 2].

Rats were fed $C_{12\text{-}14}AE_7$ in the diet at concentrations of 0%, 0.0313%, 0.0625%, 0.125%, 0.25%, 0.5% and 1.0% for 90 days. The animals in the $\geq$0.25% groups showed significantly reduced body weight gain, which was associated with marked decreases in food and water consumption. Relative liver weights were significantly increased in the $\geq$0.5% male rats and $\geq$0.25% females. Histopathologic examination showed hepatocytic enlargement in the $\geq$0.125% groups, suggesting increased liver metabolism on the basis of increased alkaline phosphatase activity at the higher dose levels. The NOAEL was established at 0.0625% in the diet or 110 mg/kg-day (HERA, 2009) [Kl. score = 2].

Rats were given in their diet 0%, 0.1%, 0.5% or 1% $C_{12-13}AE_{6.5}$ for two years. Body weight gain was reduced in the 1% males and ≥0.5% females, which was likely due to the reduced food consumption in these animals. At study termination, organ to body weight ratios were increased in the ≥0.5% females (liver, kidney and brain), 1% females (heart), and 1% males (liver). A dose-related focal myocarditis was observed in males. While focal myocarditis is commonly observed in non-treated aging rats, the incidence in the treated animals were higher than in the controls. The NOAEL was established at 0.1% or 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Inhalation

No studies are available.

Dermal

No adequate studies are available.

F. Genotoxicity

In Vitro Studies

The genotoxicity studies conducted on alcohol ethoxylates are reviewed in HERA (2009). The results of few of the *in vitro* studies on similar alcohol ethoxylates to isotridecanol, ethoxylated are presented in Table 3.

Table 3 *In Vitro* Genotoxicity Studies on Selected Alcohol Ethoxylates

Test Substance	Test System	Results*		Klimisch Score	References
		-S9	+S9		
$C_{14-15}AE_7$	Bacterial reverse mutation (*S. typhimurium* strains)	-	-	2	HERA, 2009
$C_{14-15}AE_7$	Bacterial reverse mutation (*S. typhimurium* strains)	-	-	2	HERA, 2009
$C_{14}AE_{12}$	Chromosomal aberrations (CHO cells)	-	-	2	HERA, 2009

*+, positive; -, negative

In Vivo Studies

In two separate studies, CD-1 mice were given an intraperitoneal dose of 0, 50, or 100 mg/kg $C_{12-15}AE_3$ or $C_{12-14}AE_9$. There were no increases in the frequency of micronuclei in the bone marrow cells (Talmage, 1994) [Kl. score = 2].

Male and female Tunstall rats were given a single oral gavage dose of 0, 250, 500, or 1,000 mg/kg $C_{14-15}AE_7$. There were no increases in chromosomal aberrations in the bone marrow cells (HERA, 2009) [Kl. score = 2].

G. Carcinogenicity

No studies are available on isotridecanol, ethoxylated.

Male and female Sprague-Dawley rats were given in their diet $C_{12\text{-}13}AE_{6.5}$ in the diet at doses up to 1% (500 mg/kg-day). Reduced food consumption was noted at the higher dose levels (*i.e.*, 0.5% and 1% for females and 1% for males), resulting in a lower body weight gain compared to the control group. No treatment-related histopathology was found and no increase in tumour incidence was observed (HERA, 2009) [Kl. score = 2].

Male and female Charles River rats were given in their diet 0, 0.1, 0.5 or 1% $C_{14\text{-}15}AE_7$ for two years. There were no treatment-related changes in general behaviour and appearance. The survival rate of the test animals was comparable if not better than the controls. Body weights of the 0.5% females and the 1% males and females had significantly lower weight gains than the control. There were no treatment-related effects on organ weights and tumour incidence (HERA, 2009) [Kl. score = 2]

Male and female Sprague-Dawley rats were given in their diet $C_{14\text{-}15}AE_7$ at 0.1%, 0.5% and 1% for two years. A treatment-related body weight depression was observed in females at the two highest treatment levels and in males at the 1% dose level, probably due to the poor palatability of the diet. There was no evidence for any carcinogenic activity (HERA, 2009) [Kl. score = 2].

H. Reproductive Toxicity

No studies are available on isotridecanol, ethoxylated.

CD rats were given in their diet 0%, 0.05%, 0.1% or 0.5% (approximately 0, 25, 50 or 250 mg/kg-day) $C_{12}AE_6$ in a two-generation reproductive toxicity study. There were no treatment related effects in the parents or pups on general behaviour, appearance or survival. At 0.5%, there was reduced weight gain in both the parental animals and the pups compared to the controls. Fertility was unaffected by treatment. The NOAEL for reproductive toxicity is 0.5% in the diet, which corresponds to 250 mg/kg-day (HERA, 2009) [Kl. score = 2].

In a two-generation developmental and teratogenicity study, CD rats were given in their diet 0%, 0.05%, 0.1% or 0.5% $C_{14\text{-}15}AE_7$ (approximately 0, 25, 50 or 250 mg/kg-day). Three of the treated groups were given the test substance continuously throughout the study; in the other three groups the females received the test substance on GD 6-15 and the males were untreated. None of the deaths of parental rats during the study was considered to be compound-related. There were no treatment-related changes in behaviour or appearance in the parental rats or pups. Slightly lower body weight gain was noted in the 0.5% continuously treated females. Food consumption was similar for control and treated rats. Fertility, gestation and viability indices were similar across groups. The average 21-day body weights for the 0.5% continuous treated pups were significantly lower than that of the control. Relative liver weights of the 0.5% continuously treated F_1 parental animals were increased at the 91-day sacrifice; relative liver weights of the 0.5% continuously treated males were also increased at the 60-day and caesarean section sacrifices. There were no treatment-related histopathological lesions in any of the tissues from the F_0 and F_1 generations. The NOAEL for reproductive toxicity is 0.5% in the diet or 250 mg/kg-day (HERA, 2009) [Kl. score = 2].

I. Developmental Toxicity

No studies are available on isotridecanol, ethoxylated.

In a two-generation reproductive toxicity study, Charles River rats were given in their diet 0, 0.05, 0.1 or 0.5% (about 0, 25, 50 or 250 mg/kg-day) $C_{12}AE_6$. General behaviour, appearance and survival were unaffected by treatment. At the 0.5% dose level, adults and pups gained less weight than the control rats. In the 0.5% dose group, there was a statistical increase in embryo lethality and soft tissue anomalies, and at the 0.1% there was a statistical decrease in mean foetal liver weight. Neither of these effects was considered to be treatment-related by the authors as they showed no dose response characteristics. The NOAEL for maternal toxicity is 50 mg/kg-day. The NOAEL for developmental and teratogenicity is 0.1% in the diet or 50 mg/kg-day (HERA, 2009) [Kl. score = 2].

Pregnant rabbits were given by oral gavage 0, 50, 100 or 200 mg/kg $C_{12}AE_6$ from gestational days 2 to 16. Nine control rabbits and 31 treated rabbits died during the study. Surviving rabbits at the 200 mg/kg dose group generally showed slight losses of body weight. At 100 and 200 mg/kg, ataxia and a slight decrease in body weight was observed in the pregnant animals. In seven treated and two control rabbits, early deliveries were recorded. There were no treatment-related effects on corpora lutea, implantations, number of live foetuses and spontaneous abortions. The NOAEL for maternal toxicity is 50 mg/kg-day; the NOAEL for developmental toxicity is 200 mg/kg-day (HERA, 2009) [Kl. score = 2].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for isotridecanol, ethoxylated follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

A two-year dietary study in rats has been conducted on $C_{12\text{-}13}AE_{6.5}$ (HERA, 2009). The NOAEL from this study is 50 mg/kg-day based on increased organ weights. The NOAEL of 50 mg/kg-day will be used to derive an oral reference dose and drinking water guidance value for isotridecanol, ethoxylated.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 50/(10 x 10 x 1 x 1 x 1) = 50/100 = 0.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.5 x 70 x 0.1)/2 = 1.8 mg/L

Cancer

The alcohol ethoxylates $C_{12\text{-}13}AE_{6.5}$ and $C_{14\text{-}15}AE_{7}$ were not carcinogenic to rats in a two-year dietary study. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Isotridecanol, ethoxylated does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Isotridecanol, ethoxylated has moderate chronic toxicity concern to aquatic life.

B. Aquatic Toxicity

In developing a water quality guideline for alcohol ethoxylates ANZG (2018), the toxicity data was normalised for a specific alkyl chain length or a specific number of ethoxylate (EO) groups. The NOECs listed below were normalised to an alkyl chain length of C13.3 and EO of 8.2.

Freshwater fish: 2 species, 720 to 1,500 μg/L.

Freshwater crustaceans: 2 species, 590 to 860 μg/L.

Freshwater rotifers: 1 species, *Brachionus calyciflorus*, 1,300 μg/L

Freshwater algae, diatoms and blue-green algae: 6 species, 200 to 8,700 μg/L.

Freshwater mesocosms: 4 NOEC data for multiple species tests were 80, 80, 320, and 330 μg/L, although replication was insufficient to meet OECD (1992) requirements. Normalised data were 380, 380, 320, and 1,520 μg/L.

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

$PNEC_{water}$: The ANZG water quality guideline (2018) for freshwater is: "A high reliability trigger value of 140 μg/L was derived for AE (normalised data) using the statistical distribution method with 95% protection."

For the purposes of calculating the PNEC values for sediment and soil, the $PNEC_{water}$ will be 0.14 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.71 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (6.53/1280) \times 1000 \times 0.14$
$= 0.71$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times (Kp_{sed}/1000) \times BD_{solid}]$
$= 0.8 + [0.2 \times (11.94/1000) \times 2400]$
$= 6.53\ m^3/m^3$

And:

Kp_{sed} = solid-water partition coefficient (L/kg).

BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
= 298.6 x 0.04
= 11.94 L/kg

Where:

K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for isotridecanol, ethoxylated is 298.6 L/kg.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.56 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
= (5.97/1500) x 1000 x 0.14
= 0.56 mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$Kp_{soil} = K_{oc} \times f_{oc}$
= 298.6 x 0.02
= 5.97 m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for isotridecanol, ethoxylated is 298.6 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Isotridecanol, ethoxylated is readily biodegradable and thus does not meet the screening criteria for persistence.

The bioconcentration factors (BCF) in fish for ethoxylated alcohols (which includes isotridecanol, ethoxylated) have been reported to range from <5 to 387.5. Thus, isotridecanol, ethoxylated does not meet the screening criteria for bioaccumulation.

The chronic NOEC values for alcohols ethoxylates are >0.1 mg/L. Thus, isotridecanol, ethoxylated alcohol does not meet the criteria for toxicity.

The overall conclusion is that isotridecanol, ethoxylated is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for isotridecanol, ethoxylated.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Isotridecanol, ethoxylated	69011-36-5	Not a PBT	No	No	No	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AE	alcohol ethoxylates
AES	alcohol ethoxy sulphates
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Environment Guidelines
ARMCANZ	Agriculture and Resource Management Council of Australia and New Zealand
BCF	bioconcentration factor
CAS	Chemical Abstracts Service
CHO	Chinese hamster ovary
COC	constituent of concern
DEWHAD	Department of Environment, Water, Heritage and the Arts
DoEE	Department of Environment and Energy
ECHA	European Chemicals Agency
EO	ethoxylate
EU	European Union
g/L	grams per litre
GD	gestational day
GHS	Globally Harmonized System of Classification and Labelling of Chemicals
HERA	Human and Environmental Risk Assessment
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/d	kilograms per day
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration

LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mm^2/s	square millimetres per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
µg/L	micrograms per litre

Attachment 2 Mass Balance Calculations

Attachment 2
Summary of Exposure Point Concentration Development
(Initial and Underbalance Workover Fluid Chemicals)

Mass Balance

In other Santos project areas, approximately 1,540 mg/L of the product is being dosed (5 L of product added to 3,250 litres of water) during each well treatment. The product dose is apportioned between the constituents of potential concern (COPCs) based on the COPC percent weight in the product (composition information in the safety data sheet) for COPC dosage rate per well. The eight-well COPC flowback concentrations are calculated based on the treatment of eight wells per day, and dilution by produced water (3,250 L) during well flush. The concentration of the COPCs in the water storage pond influent was based on dilution from the combined average field and groundwater bore water productions (0.5 ML/d).

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	Dosage Rate per Well (mg/L)	8-Well Flowback (mg/L)	Storage Pond Influent (mg/L)
Isotridecanol, ethoxylated	69011-36-5	3.3	51	1.2E-01	2.2E-07

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
mg/L = milligrams per litre

Qualitative Tier 2 Assessment

Monoethanolamine

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme1 is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Monoethanolamine is a component in a drilling fluid product used for pH control in the following fluid systems: Inhibitive Mud System and Inhibited Star Shield Mud System. The first fluid system is one of the primary systems to be used as drilling fluids. The Inhibited Star Shield mud system is used as a preventative wellbore shielding additive during drilling operations for the production of coal seam gas.

The purpose and maximum quantity (i.e., in all muds) for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Monoethanolamine	141-43-5	pH control	NA

[1] Based on maximum of combined muds assessed
CAS No = Chemical Abstracts Service Number
NA = Not available

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no adequate or reliable carcinogenic studies available for monoethanolamine; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Monoethanolamine (141-43-5)	2-year rat dietary reproduction	General Systemic Toxicity	300	300	1	3.5

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Monoethanolamine (141-43-5)	Algae	0.70	10	0.07

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Monoethanolamine (141-43-5)	[a]	-	-	0.060

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Monoethanolamine (141-43-5)	[a]	-	-	0.014

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Monoethanolamine is a clear liquid with a fish odour. The molecular structure for monoethanolamine is presented in **Figure 1**.

Figure 1 Molecular Structure of Monoethanolamine[2]

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/141-43-5

Monoethanolamine is highly soluble in water. The measured pKa of 9.5 indicates that the substance will primarily exist as a cation in the environment. Based upon an organic carbon partition coefficient (K_{oc}) of 15 L/Kg for the charged molecule, if released to soil, monoethanolamine is not expected to adsorb to soil and has a potential for high mobility. If released into water, monoethanolamine is also not expected to adsorb to suspended solids and sediment. However, absorption is affected by the acidity of the substrate.

Monoethanolamine is readily biodegradable and is not expected to bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for monoethanolamine is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

The acute toxicity of monoethanolamine is low by the oral, dermal and inhalation routes. It is a skin and eye irritant, but it is not a skin or respiratory sensitiser. Based on the data available, the chemical is not considered to cause serious damage to health from repeated oral exposure or through inhalation. No critical effects were observed. No data are available to evaluate systemic exposure via the dermal pathway. The substance is not genotoxic when tested in both in vitro and in vivo assays. There is no indication that this substance will have an adverse effect on reproduction and development.

Based on a review of a two-year oral reproductive study in rats, TRVs were derived for monoethanolamine. The drinking water guideline value derived for monoethanolamine using the non-carcinogenic oral RfD is 3.5 mg/L (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Monoethanolamine may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to monoethanolamine in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in recovered drilling fluids would be diluted by at least 90% in the water feed pond due to the aggregation with produced water. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, monoethanolamine is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME)

now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, monoethanolamine is moderately toxic to aquatic organisms. In acute toxicity studies, algae were more sensitive compared to fish and invertebrates (ECHA). However, in chronic toxicity studies algae and invertebrates were equally sensitive (ECHA).

Monoethanolamine is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to soil.

PNECs for monoethanolamine are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs in water. However, there are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated

effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of monoethanolamine in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of monoethanolamine in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as monoethanolamine, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

MONOETHANOLAMINE

This dossier on monoethanolamine presents the most critical studies pertinent to the risk assessment of monoethanolamine in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. Most of the information presented in this dossier was obtained from the ECHA database which provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Monoethanolamine was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Monoethanolamine was assessed as a tier 2 chemical for acute and chronic toxicity. Therefore, monoethanolamine is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Monoethanolamine is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to soil. The acute toxicity of monoethanolamine is low by the oral, dermal and inhalation routes. It is a skin and eye irritant, but it is not a skin or respiratory sensitiser. Based on the data available, the chemical is not considered to cause serious damage to health from repeated oral exposure or through inhalation. No critical effects were observed. No data are available to evaluate systemic exposure via the dermal pathway. The substance is not genotoxic when tested in both *in vitro* and *in vivo* assays. There is no indication that this substance will have an adverse effect on reproduction and development. Monoethanolamine has moderate toxicity to aquatic organisms based on chronic studies.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2-aminoethanol

CAS RN: 141-43-5

Molecular formula: C_2H_7NO

Molecular weight: 61.08 g/mol

Synonyms: Monoethanolamine; MEA; ethanolamine

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Monoethanolamine

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear liquid with fish odour	2	ECHA
Melting Point	4 °C	2	ECHA
Boiling Point	167 °C @ 101.3 kPa	2	ECHA
Density	1016 kg/m^3 @ 20 °C	2	ECHA
Vapor Pressure	50 Pa @ 20 °C	2	ECHA
Partition Coefficient (log K_{ow})	-2.3 @ 25 °C	2	ECHA
Water Solubility	>1000 g/L @ 20 °C (pH 12.1)	2	ECHA
Dissociation Constant (pKa)	9.5 @ 25 °C	2	ECHA
Viscosity	23.86 mPa·s (dynamic) @ 20 °C	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for monoethanolamine.

NICNAS has assessed monoethanolamine in an IMAP Tier 1 assessment and it was concluded that this chemical poses no unreasonable risk to the environment[1].

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=141-43-5

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Monoethanolamine is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to soil.

B. Partitioning

Monoethanolamine is highly soluble in water. A pKa of 9.5 indicates monoethanolamine will exist almost entirely in the cation form at pH values of 5 to 9 and, therefore, volatilization from water surfaces is not expected to be an important fate process. Likewise, volatilization from moist soil is not expected because cations do not volatilize. Monoethanolamine is not expected to volatilize from dry soil surfaces based upon its vapor pressure.

Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyse under environmental conditions (pH 5 to 9) (PubChem).

C. Biodegradation

Monoethanolamine is considered readily biodegradable. In OECD 301A test, degradation was found to be > 90% after 21 days (ECHA) [KI. Score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No reliable experimental data are available for monoethanolamine. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from log K_{ow} is 0.166 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 1.2 L/kg. Both estimates refer to the uncharged molecule. While the substance was completely inside the applicability domain of the MCI model, the log K_{ow} of monoethanolamine was slightly outside of the range of the training set of the K_{ow} method. Therefore, the estimate of the log K_{ow} method may be less accurate. (ECHA) [KI. Score = 2].

The measured pKa of 9.5 indicates that the substance will primarily exist as a cation in the environment. Cations generally adsorb stronger to soils containing organic carbon and clay than their neutral counterparts. Franco & Trapp (2008, 2009, 2010) have developed a method to take this effect into consideration when assessing the adsorption potential. The model is not yet validated; in addition, the applicability domain is not clearly defined. Nevertheless, the K_{oc} values of the Franco & Trapp method give a good indication on the adsorption potential of a substance depending on the pH conditions of soil. The method is based on the dissociation constant pKa and the log K_{ow} for the uncharged molecule. Regarding the charged molecule, at pH 7 the log K_{oc} was estimated to be 1.16 (K_{oc} = 15 L/kg) following the method of Franco & Trapp (2008, 2009, 2010) based on a pKa value of 9.5 and a log K_{ow} value of -1.61. (ECHA) [KI. Score = 2].

Based upon these K_{oc} values, if released to soil, monoethanolamine is not expected to adsorb to soil and has a potential for high mobility. If released into water, monoethanolamine is also not expected

to adsorb to suspended solids and sediment. However, absorption is affected by the acidity of the substrate (PubChem).

E. Bioaccumulation

A QSAR study using OASIS Catalogic v 5.13.1 [BCF base line model-v.03.10] was used to derive a bioaccumulation factor (BCF) of 2.5 L/kg which considers all mitigating factors. A BCF value of 9.2 was derived assuming no mitigating factors. (ECHA)[KI. Score=2] These BCF values suggests that monoethanolamine is not expected to bioaccumulate, which is consistent with a log K_{ow} of -2.3 (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of monoethanolamine is low by the oral, dermal and inhalation routes. It is a skin and eye irritant, but it is not a skin or respiratory sensitiser. Based on the data available, the chemical is not considered to cause serious damage to health from repeated oral exposure or through inhalation. No critical effects were observed. No data are available to evaluate systemic exposure via the dermal pathway. The substance is not genotoxic when tested in both *in vitro* and *in vivo* assays. There is no indication that this substance will have an adverse effect on reproduction and development.

B. Toxicokinetics

There are no studies available to determine the toxicokinetics of monoethanolamine via the oral or inhalation routes of exposure. *In vivo* studies using radioactive monoethanolamine, show that it penetrates the skin and then it is widely distributed throughout the body. More specifically 24% of the radioactive dose was found in the liver, 24.3% on skin, 18% exhaled CO_2, 4.6% urine, 2.5% kidneys, and 1.8% feces. (ECHA) [KI. Score =2].Transdermal uptake was determined to be slower than intraperitoneal administration. In short, monoethanolamine is readily metabolized in the skin and other organs with the liver being the target organ for metabolism. Dermal absorption for workers and consumers is 37.5% and 75% respectively.

C. Acute Toxicity

In an OECD Guideline 401 (Acute oral Toxicity) study, the oral LD_{50} value in rats was found to be 1089 mg/kg/bw for males and females (ECHA) [KI. Score =2].

LC_{50} values of 1487 mg/m^3 (4 hours) and >1300 mg/m^3 (6 hours) was determined for acute inhalation toxicity in rats (ECHA) [KI. Score =2].

In an OECD Guideline 402 (Acute Dermal Toxicity) study, the dermal LD_{50} in rabbits was found to be 2504 mg/kg/bw (ECHA) [KI. Score = 2].

D. Irritation

In an OECD Guideline 404 (Acute Dermal Irritation/Corrosion) study, monoethanolamine was found to be corrosive to rabbits with irreversible effects after 8 days of exposure (ECHA) [KI. Score =2).

In an OECD Guideline 405 (Acute Eye Irritation/ Corrosion) study, monoethanolamine was found to be corrosive to the eyes of rabbits with irreversible effects after 8 days of exposure (ECHA) [KI. Score =2]. The mean of the 24-, 48-, and 72-hour scores were: 3 for corneal opacity, 0.88 iridial lesions, 0.89 conjunctival redness, and 1.33 chemosis.

E. Sensitisation

Monoethanolamine was identified as a not sensitising in a guinea pig maximisation test after 48h and 72 h readings (ECHA) [KI.Score =2).

A respiratory sensitisation test (bronchoconstriction [Pao] and analysis of Histamine in Bronchoalveolar Lavage Fluid [BALF]) in guinea pigs did not identify an adverse effect (not sensitising) following exposure to monethanolamine (ECHA)[KI.Score =2].

F. Repeated Dose Toxicity

Oral

Read-across substance monoethanolamine HCI was tested in a two-generation reproduction toxicity study as per an OECD Guideline 416. The F0 parental generation consisted of 25 Male and 25 female Wistar rats that were fed monoethanolamine HCI at the following doses: 0, 100,300, and 1000 mg/kg/bw/day. After 75 days of treatment the F0 animals were mated to produce a litter (F1 generation). There were no adverse effects were observed in the 100 and 300 mg/kg F0 and F1 parental animals. Systemic toxicity, in parental females, was characterized by lowered food consumption and/or body weight during gestation and lactation. The absolute and relative kidney weights were significantly increased without corresponding histopathological findings in the F1 animals dosed at 300 mg/kg/bw/day. The kidneys of all the treated males and females showed a low incidence of basophilic tubules in a slightly higher number of animals compared to the controls. The severity (minimal to slight) was comparable between treated, and controls and a clear dose-response relationship was not observed. The no observed adverse effect level (NOAEL) for general toxicity is 300 mg/kg-day (ECHA) [KI. score = 1].

Inhalation

In an OECD Guideline 412 (Subacute Inhalation Toxicity: 28-day Study) study, five male and five female Wistar rats were exposed by inhalation (nose-only) to 0, 10, 50, or 150 mg/m^3 monoethanolamine aerosol, 6 hours/day, 5 days/week for 28 days (20 exposures). The mean mass aerodynamics diameters (MMADs) in the 150 mg/m^3 group were 1.1 and 1.2 μm with a GSD of 5.3 and 5.4. The calculated mass fractions of particles <3 μm aerodynamic size were 70.0% and 70.3%, respectively. There were no effects that were considered to be from systemic exposure. Histopathological effects were seen in the larynx, trachea, and lung; these effects were considered to be site-of-contact effects from the irritating nature of the test material. The no observed adverse effect concentration (NOAEC) for systemic toxicity is 150 mg/m^3, the highest exposure concentration tested. The lowest observed adverse effect concentration (LOAEC) for localized (irritation) effects is 10 mg/m^3; a NOAEC was not determined (ECHA) [KI. score = 1]

Dermal

There are no adequate or reliable studies available.

G. Genotoxicity

In Vitro Studies

The results of the *in vitro* genotoxicity studies on monoethanolamine are presented in Table 3.

Table 3 *In Vitro* Genotoxicity Studies on 2-Ethylhexanol

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Mammalian cell gene mutation (Chinese hamster lung fibroblasts, V79)	-	-	2	ECHA
Chromosome aberration study in mammalian cells (Rat hepatocytes, RL4)	-	-	2	ECHA
Gene mutation study in mammalian cells (mouse lymphoma L5178 Y cells)	-	-	1	ECHA
Gene mutation study in bacteria (S. typhimurium and E. coli strains)	-	-	1	ECHA

*+, positive; -, negative

In Vivo Studies

In an OECD guideline 474 (Mammalian Erythrocyte Micronucleus Test) study, five male and five female Naval Medical Research Institute (NMRI) mice, at each dose level, received monoethanolamine on two consecutive days at the following doses, oral gavage, 0, 375, 750, or 1,500 mg/kg. There were no biologically relevant or statistical differences observed in the frequency of micronucleated polychromatic erythrocytes in the treated mice when compared to the controls (ECHA) [Kl. score = 1].

H. Carcinogenicity

Oral

There are no adequate or reliable carcinogenicity studies available.

Inhalation

No studies are available.

I. Reproductive Toxicity

In an OECD Guideline 416 (Two-Generation Reproduction Toxicity Study) study, male and female Crl:WI (Han) rats were fed in their diet 0, 100, 300, or 1,000 mg/kg methanolamine. There were no adverse effects seen in the 100 and 300 mg/kg F0 and F1 parental animals. Feed consumption was lower in the 1,000 mg/kg F0 females during lactation. Body weight gain and, for the F0 generation, body weights of the 1,000 mg/kg dams were significantly lower during gestation, which was considered to be secondary to increased post-implantation loss in these animals. At 1,000 mg/kg, absolute and relative epididymides and cauda epididymidis weights were reduced and,

in the F0 generation only, the number of homogenization resistant caudal epididymal sperm was slightly, but significantly, reduced. There was no accompanying histopathogical findings. In the F0 and F1 1,000 mg/kg females, the numbers of implants were decreased and the resorption rates were increased, resulting in significantly smaller litters. There were no other treatment-related effects on the reproductive parameters measured. There were no indications for any developmental toxicity in the F1 and F2 offspring. The NOAEL for systemic toxicity and fertility and reproductive performance is 300 mg/kg-day. The NOAEL for pre- and post-natal developmental toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

Moore and co-workers investigated the potential role of choline antagonism in the aetiology of monoethanolamine (MEA)-induced implantation loss. When administered to pregnant rats during gestation days (GD) 1–3, 4–5, or 6–7, MEA had no effect upon implantation success. In a second experiment, MEA was administered either in the diet or by oral gavage from two weeks prior to mating through to GD 8. Parallel groups also received a diet supplemented with choline. In the absence of supplementary choline, MEA induced early resorptions, statistically significant only when administered in the diet. A slight reduction in implantation success was ameliorated by supplementary choline. It was concluded that implantation is affected by MEA only when exposure starts before mating; that dietary administration is more effective than gavage dosing; and that interference with choline homeostasis may play a role in the aetiology of this lesion (ECHA). [Kl. score = 1] Rodents appear to be more sensitive towards effects on choline homeostasis and effects observed have been assessed to lack human relevance (ECHA).

J. Developmental Toxicity

Oral

In an OECD Guideline 414 (Prenatal Developmental Toxicity Study) study, pregnant female Wistar rats were dosed by oral gavage with 0, 40, 120, or 450 mg/kg monoethanolamine on GD 6-15. Feed consumption, lower mean body weights and reduced body weight gain was observed in the 450 mg/kg dams. There was no developmental toxicity. The NOAEL for maternal is 120 mg/kg-day; the NOAEL for developmental toxicity is 450 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 1].

Inhalation

No adequate and reliable studies available.

Dermal

In an OECD Guideline 414 (Prenatal Developmental Toxicity Study) study, pregnant female New Zealand White rabbits were given dermal applications of 0, 10, 25, and 75 mg/kg monoethanolamine 6 hours/day on GD 6-18. There was severe skin irritation at the site of exposure in the 75 mg/kg animals. Skin irritation was also observed in some of the 25 mg/kg females, but to a much less degree of severity. There were no other maternal toxic effects. There was no developmental toxicity. The NOAEL for maternal toxicity is 10 mg/kg-day; the NOAEL for developmental toxicity is 75 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 2].

Pregnant female SD rats were given dermal applications of 0, 10, 25, 75, or 225 mg/kg monoethanolamine 6 hours/day on GD 6-15. In the 225 mg/kg group, there was skin irritation at the site of application and body weight gain was reduced during the exposure period. There was no

developmental toxicity. The NOAEL for maternal toxicity is 75 mg/kg-day; the NOAEL for developmental toxicity is 225 mg/kg-day, the highest dose tested (ECHA) [Kl. score = 2]

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for monoethanolamine follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

In a two-generation oral reproductive toxicity study, there was reduced food consumption and/or body weight gain, as well as organ weight changes unaccompanied by histopathological findings, in the male and female rats fed 1,000 mg/kg-day monoethanolamine. The NOAEL for general systemic toxicity was set at 300 mg/kg-day from this study. The NOAEL of 300 mg/kg-day will be used to determine the oral reference dose and drinking water guidance value for monoethanolamine.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 300/(10 x 10 x 1 x 3 x 1) = 300/300 = 1 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (1 x 70 x 0.1)/2 = 3.5 mg/L

Cancer

There are no adequate or reliable carcinogenic studies available for monoethanolamine. Therefore, a cancer reference value was not derived.

L. Human Health Hazard Assessment of Physico-Chemical Properties

Monoethanolamine does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Monoethanolamine has moderate toxicity to aquatic organisms based on chronic studies.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on monoethanolamine.

Table 4 Acute Aquatic Toxicity Studies on Monoethanolamine

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss (Rainbow Trout)	96-hour LC_{50}	105	2	ECHA
Cyprinus carpio (Common Carp)	96-hour LC_{50}	349	1	ECHA
Oryzias latipes (Medaka)	96-hour LC_{50}	> 100	2	ECHA
Pimephales promelas (Fathead Minnow)	96-hour LC_{50}	2070	2	ECHA
Carassius auratus (goldfish)	96-hour LC_{50}	170	2	ECHA
Danio rerio (zebrafish)	96-hour LC_{50}	3682	2	ECHA
Daphnia magna	48-hour EC_{50}	27	1	ECHA
Pseudokirchneriella subcapitata	72-hour EC_{50}	2.80	2	ECHA

Chronic Studies

A 41-day NOEC for Oryzias latipes (Medaka) in an OECD 210 test is 1.24 mg/L (ECHA)[KI. Score= 2].

The long-term effects on aquatic invertebrates were assessed in a 21-day chronic reproduction test on Daphnia magna, according to OECD guideline 202. The 21-day NOEC was determined to be 0.85 mg/L for reproduction (ECHA)[KI. Score = 2].

Monoethanolamine has been evaluated for its toxicity towards the fresh water algae *Pseudokirchneriella subcapitata* (formerly *Selenastrum capricornutum*) in an Alga growth inhibition test according to OECD 201 under GLP requirements. The exposure duration was 72 hours under static conditions. The 72-hr EC_{10} growth rate determined from the study was 0.7 mg/L (ECHA) [KI. Score = 2].

C. Terrestrial Toxicity

Indirect exposure to the soil compartment is unlikely since the substance is readily biodegradable. Consequently, no tests on soil organisms are required. However, long-term toxicity studies are available for earthworms, collembolans, and terrestrial plants. Chronic effect values (EC_{10} or NOEC) were not reported. Only EC25 and EC50 were reported, which are considered acute effect values. Acute effects data is summarized below:

A 35-day LC_{50} earthworm (*Eisenia Andrei*) - 3,715 mg/kg (mortality) (ECHA) [KI. Score = 2]

A 63-day EC_{50} earthworm - 4,033 mg/kg (reproduction)(ECHA) [KI. Score = 2]

A 63-day EC_{25} earthworm - 2,016 mg/kg (reproduction)(ECHA) [KI. Score = 2]

A 28-day LC_{50} springtails (*Folsomia candida*) 1,893 mg/kg (mortality) (ECHA) [KI. Score = 2]

A 14-day EC_{50} plants (*Hordeum vulgare*) - 2,939 mg/kg (growth, shoot dry mass) (ECHA) [KI. Score = 2]

No studies on the toxicity to birds are available for the substance.

D. Calculation of PNEC

The PNEC calculations for monoethanolamine follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (105 mg/L), invertebrates (27 mg/L), and algae (2.8 mg/L). Results from chronic studies are also available for all three trophic levels, with the lowest NOEC or EC_{10} value being 0.70 mg/L for algae. On the basis that the data consists of short-term and long-term results from three trophic levels, an assessment factor of 10 has been applied to the lowest reported EC_{10} value of 0.70 mg/L for algae. The resulting $PNEC_{water}$ is 0.07 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.060 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (1.088/1280) \times 1000 \times 0.07$
$= 0.0595$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water (mg/L) [calculated above]

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 0.6/1000 \times 2400]$
$= 1.088\ m^3/m^3$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 15 \times 0.04$
$= 0.6$ L/kg

Where:
K_{oc} = The calculated K_{oc} value for monoethanolamine is 15 L/Kg following the method of Franco & Trapp (2008, 2009, 2010) (ECHA)[KI.Score=2]
f_{oc} = fraction of organic carbon in sediment = 0.04 [default]

PNEC soil

Indirect exposure to the soil compartment is unlikely since the substance is readily biodegradable. In addition, chronic effect levels were not reported in available long-term toxicity studies. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.014 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (0.3/1500) \times 1000 \times 0.07$
$= 0.014$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]

$PNEC_{water}$ = predicted no effect concentration in water (mg/L) [calculated above]

$Kp_{soil} = K_{oc} \times f_{oc}$
= 15 x 0.02
= 0.3 m^3/m^3

Where:
K_{oc} = The calculated K_{oc} value for monoethanolamine is 15 L/Kg following the method of Franco & Trapp (2008, 2009, 2010) (ECHA)[KI.Score=2]
f_{oc} = fraction of organic carbon in soil = 0.02 [default]

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Monoethanolamine is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -2.3, monoethanolamine does not meet the screening criteria for bioaccumulation.

The chronic NOEC values for monoethanolamine are >0.1 mg/L. Thus, monoethanolamine does not meet the screening criteria for toxicity.

Therefore, monoethanolamine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for monoethanolamine.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Monoethanolamine	141-43-5	Not a PBT	No	No	No	No	No	No	1 (fish, inv) 2 (algae)	1 (fish), 2 (inv, algae)	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
BALF	Bronchoalveolar Lavage Fluid
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DoEE	Department of Environment and Energy
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
IMAP	Inventory Multitiered Assessment and Prioritisation Program
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme

NOAEC	No Observed Adverse Effect Concentration
NOAEL	No Observed Adverse Effect Level
NOEC	No Observed Effect Level
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
USEPA	United States Environmental Protection Agency

Attachment 2 Mass Balance Calculations

Attachment 2

Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
Monoethanolamine	141-43-5	5.00E+01	1.50E+01	5.00E+00	1.25E+00	5.00E-02	1.25E-02	1.00E-03	2.50E-04	7.00E-02

**Concentration based on reported %mass composition of similar products used for pH control*

Notes:

mg/L = milligrams per liter

CAS = Chemical Abstracts Service

NA = not applicable

PNEC = predicted no effects concentration

RO = reverse osmosis

WMF = Water Management Facility

Qualitative Tier 2 Assessment

Oxazolidine

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Oxazolidine is a component in a drilling fluid product used as a biocide in the KCl/Polymer Mud fluid system. The purpose and maximum quantity for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Oxazolidine	66204-44-2	Biocide	NA

[1] Based on maximum of combined muds assessed
CAS No = Chemical Abstracts Service Number
NA = Not available

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no adequate or reliable carcinogenic studies available for oxazolidine; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in **Attachment 1**. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Oxazolidine (66204-44-2)	1-generation reproductive study in rats	Reduced body weight	15	1000	0.015	0.053

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Oxazolidine (66204-44-2)	Invertebrates	1.3	50	0.026

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Oxazolidine (66204-44-2	[a]	-	-	0.017

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%

mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Oxazolidine (66204-44-2	[a]	-	-	0.00035

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Oxazolidine is a clear, colourless to yellowish liquid with an amine odour. The molecular structure for oxazolidine is presented in **Figure 1**.

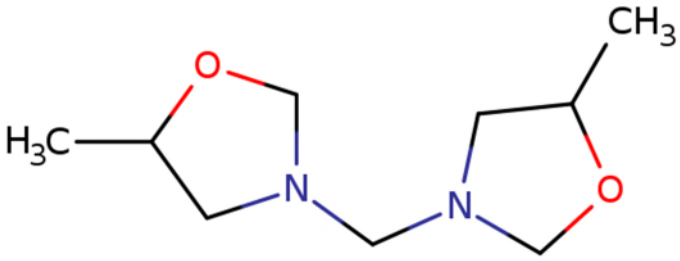

Figure 1 Molecular Structure of Oxazolidine[2]

Oxazolidine is a reaction mixture that consists of several constituents (water, formaldehyde, and 2-hydroxylpropylamine [HPA]). At room temperature, the substance is completely miscible with water. In aqueous solution, a dynamic equilibrium exists, whose composition depends on the concentration, pH value, and temperature. Thus, a precise experimental determination of the physical-chemical properties of the mixture or its constituents is difficult (ECHA).

Oxazolidine rapidly degrades in water, so this substance could not be used for analysis; therefore, the reaction product 5-methyl-oxazolidine was used as the analytical target compound. For the

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/66204-44-2

reaction compound, an organic carbon partition coefficient (K_{oc}) of 1 litre per kilogram (L/Kg) was determined. Based on this value, if released to soil, oxazolidine is not expected to adsorb to soil if released and has a potential for mobility. If released into water, it is not expected to adsorb to suspended soils or sediment based on its K_{oc} value and rapid hydrolysis.

Oxazolidine is readily biodegradable and has a low potential for bioaccumulation.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for oxazolidine is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that the substance is not a PBT substance.

Human Health Hazards

The acute toxicity of oxazolidine is moderate for oral, dermal, and inhalation routes of exposure. Depending on the concentration of the solution (neat vs. diluted) the substance is corrosive to the skin and eyes. It is also a skin sensitiser. Oxazolidine induces local effects in the stomach after repeated exposure via oral gavage. However, this effect is not considered relevant to humans. The reaction products of oxazolidine are genotoxic in *in vitro* studies but not *in vivo* studies. There are no carcinogenicity studies on oxazolidine. Assuming that the possible mutagenic and carcinogenic effects of oxazolidine are based on the hydrolysis product formaldehyde, no carcinogenic effects are expected at these threshold concentrations. There is no indication that this substance will have an adverse effect on reproduction and development.

Based on a review of a one generation oral reproductive study in rats, TRVs were derived for oxazolidine. The drinking water guideline value derived for the substance using the non-carcinogenic oral RfD is 0.053 mg/L (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

Oxazolidine may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to oxazolidine in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in recovered drilling fluids would be diluted by at least 90% in the water feed pond due to the aggregation with produced water. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, oxazolidine is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**).

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME)

now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, overall oxazolidine is moderately toxic to aquatic life. The acute toxicity of oxazolidine is of low concern to fish and invertebrates and of moderate concern to algae. The chronic toxicity of oxazolidine is of moderate concern to invertebrates and algae. Based on hazard data, invertebrates are slightly more sensitive than algae in chronic toxicity studies. (ECHA).

Oxazolidine is readily biodegradable. It is not expected to bioaccumulate, and it has low potential to adsorb to soil.

PNECs for oxazolidine are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs in water. However, there are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre

(ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of oxazolidine in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of oxazolidine in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as oxazolidine, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days. This is a conservative assumption as biodegradation studies detailed in the dossier provided in **Attachment 1** indicated greater degradation in a less time (i.e., >60% after 4 days). In addition, this chemical is also subject to hydrolysis (half-life of <4 hours).

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the hSantos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

References

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Attachment 1 Risk Assessment Dossier

Oxazolidine

This dossier on oxazolidine presents the most critical studies pertinent to the risk assessment of oxazolidine in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Oxazolidine was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Oxazolidine was assessed as a tier 2 chemical for acute toxicity and as a tier 1 for chronic toxicity. Therefore, this substance is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Oxazolidine is an organic UVCB (Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials) substance. This substance undergoes hydrolysis, and its reaction products are formaldehyde and 2-hydroxylpropylamine (HPA).

Oxazolidine is readily biodegradable. This substance is completely hydrolysed in the environment and as a result, has a low potential for bioaccumulation. Likewise, it is expected to adsorb very little to soil, suspended solids, or sediment.

The acute toxicity of oxazolidine is moderate for oral, dermal, and inhalation routes of exposure. Depending on the concentration of the solution (neat vs. diluted), oxazolidine is corrosive to the skin and eyes. It is also a skin sensitiser. Oxazolidine induces local effects in the stomach after repeated exposure via oral gavage. However, this effect is not considered relevant to humans. The reaction products of oxazolidine are genotoxic in *in vitro* studies but not *in vivo* studies. There are no carcinogenicity studies on oxazolidine. Assuming that the possible mutagenic and carcinogenic effects of oxazolidine are based on the hydrolysis product formaldehyde, no carcinogenic effects are expected at these threshold concentrations. There is no evidence for adverse effects of the substance on embryo and foetal development at dose levels inducing no local maternal toxicity.

Overall, oxazolidine is moderately toxic to aquatic life.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 5-methyl-3-[(5-methyl-1,3-oxazolidin-3-yl) methyl]-1,3-oxazolidine

CAS NO.:66204-44-2

Molecular formula: $C_9H_{18}N_2O_2$

Molecular weight: 186.25 g/mol

Synonyms: Oxazolidine, 3,3'-methylenebis[5-methyl-;3,3'-Methylenebis(5-methyloxazolidine); 3,3'-METHYLENEBIS[5-METHYLOXAZOLIDINE];5-methyl-3-[(5-methyl-1,3-oxazolidin-3-yl)methyl]-1,3-oxazolidine

3 PHYSICO-CHEMICAL PROPERTIES

Oxazolidine is a reaction mixture that consists of several constituents (water, formaldehyde, and HPA). At room temperature, the substance is completely miscible with water. In aqueous solution, a dynamic equilibrium exists, whose composition depends on the concentration, pH value, and temperature. Thus, a precise experimental determination of the physical-chemical properties of the mixture or its constituents is difficult (ECHA). Key physical and chemical properties for the substance are shown in **Table 1**.

Table 1: Overview of the Physico-Chemical Properties of Oxazolidine

Property	Value	Klimisch Score	Reference
Physical state at 20 °C and 101.3 kPa	Clear, colourless to yellowish liquid with an amine odour	2	ECHA
Melting Point	-60.5 °C @ 101.3 kPa	1	ECHA
Boiling Point	192.2 °C @ 101.3 kPa	1	ECHA
Density	1.05 (relative density) @ 20 °C	1	ECHA
Vapor Pressure	1.4 Pa @ 25 °C	2	ECHA
Partition Coefficient (log K_{ow})	-0.043temperature not provided	1	ECHA
Water Solubility	Completely miscible at room temperature	1	ECHA
Dissociation constant (pKa)	pKa determination not possible due to hydrolysis	1	ECHA
Viscosity	21 mPa s @ 20 °C	2	ECHA

kPa = kilopascal
°C = degrees Celsius
mPa = Megapascal
s = second
ECHA = European Chemicals Agency

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances (AICS; Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for oxazolidine.

Table 2 Existing International Controls

Convention, Protocol, or Other International Control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No

Convention, Protocol, or Other International Control	Listed Yes or No?
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Oxazolidine is readily biodegradable. This substance is completely hydrolysed in the environment and as a result, has a low potential for bioaccumulation. Likewise, it is expected to adsorb very little to soil, suspended solids, or sediment.

B. Partitioning

Oxazolidine is water soluble, and it is not expected to be volatile from aqueous solutions. This substance is completely hydrolysed in the environment, and its reaction products are formaldehyde and HPA. The reaction rate of hydrolysis was determined at different pH values via measurement of the formaldehyde being released. At pH 4 and 7, the formaldehyde content reached a plateau after approximately 1-2 hours, while the reaction was slightly slower at pH 9, reaching the plateau after 3-4 hours (ECHA). [KI. Score = 1].

C. Biodegradation

As per OECD Test Guideline 301 B (Ready Biodegradability: CO2 Evolution Test), there was 66.1% degradation after 4 days and 89.8% degradation after 28 days (ECHA). [KI score =1]. These results indicate that oxazolidine is readily biodegradable. In short, this substance and its hydrolysis products are expected to be extensively removed in biological treatment plants, as well as in aquatic compartments.

If a chemical is found to be readily biodegradable, it is categorized as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

Oxazolidine rapidly degrades in water, so this substance could not be used for analysis; therefore, the reaction product 5-methyl-oxazolidine was used as the analytical target compound. As per OECD Test Guideline 121, the upper limit organic carbon to water partition coefficient (K_{oc}) value was estimated to be ≤1 litres per kilogram (L/kg; ECHA). [KI score =1]

Based on this K_{oc} value, oxazolidine is not expected to adsorb to soil if released and has a high mobility. If oxazolidine is released to water, it is not expected to adsorb to suspended soils or sediment based on its K_{oc} value and rapid hydrolysis.

E. Bioaccumulation

There are no bioaccumulation studies on oxazolidine. Therefore, quantitative structure-activity relationship (QSAR) models were used to calculate values for the bioconcentration factor (BCF) in earthworms (0.96 L/kg) and fish (1.41 L/kg) (ECHA). [Kl. Score = 1]. Based on these values, low potential for bioaccumulation is expected. Furthermore, the constituents of the reaction product hydrolyse in aqueous media.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of oxazolidine is moderate for oral, dermal, and inhalation routes of exposure. Depending on the concentration of the solution (neat vs. diluted) oxazolidine is corrosive to the skin and eyes. It is also a skin sensitiser. Oxazolidine induces local effects in the stomach after repeated exposure via oral gavage. However, this effect is not considered relevant to humans. The reaction products of oxazolidine are genotoxic in *in vitro* studies but not *in vivo* studies. There are no carcinogenicity studies on oxazolidine. Assuming that the possible mutagenic and carcinogenic effects of oxazolidine are based on the hydrolysis product formaldehyde, no carcinogenic effects are expected at these threshold concentrations. There is no evidence for adverse effects of the substance on embryo and foetal development at dose levels inducing no local maternal toxicity.

B. Toxicokinetics

Oxazolidine undergoes hydrolysis, which results in formaldehyde and 5-methyloxazolidine as reaction products. Toxicokinetic data could not be obtained on the parent compound because it is a complex mixture. However, data on formaldehyde is available considering that this is the most toxicologically important constituent of the mixture.

In rats, the dermal absorption for formaldehyde is 30-40%. The inhalation absorption for formaldehyde is 90% in rats, 67% in Monkeys, and 76% in humans. The oral absorption for formaldehyde in rats and mice has limited validity. Formaldehyde is rapidly oxidized to formic acid then it enters the carbon-1-metabolic pathway. Formic acid can also be cleaved to CO_2 and exhaled, or it can be excreted in the form of sodium formate via urine (ECHA). [KI Score =1].

C. Acute Toxicity

<u>Oral</u>

As per OECD Test Guideline 423 (Acute Oral Toxicity-Acute Toxic Class Method) and EU Method B.1 tris (Acute Oral Toxicity-Acute Toxic Class Method), the LD_{50} in male and female rats was determined to be 630 milligrams per kilogram bodyweight (mg/kg bw) (ECHA). [KI.score =1].

<u>Dermal</u>

As per OECD Test Guideline 402 (Acute Dermal Toxicity) and EU Method B.3 (Acute Toxicity Dermal), the LD_{50} in female rats was determined to be ≥760 mg/kg bw (ECHA). [KI score=1].

Inhalation

As per OECD Test Guideline 436 (Acute Inhalation Toxicity: Acute Toxic Class Method), the LC_{50} in male and female rats was determined to be > 1000 milligrams per cubic metre (mg/m^3;nominal) (ECHA). [KI score =1].

D. Irritation

Skin

As per OECD Test Guideline 404 (Acute Dermal Irritation/Corrosion) and EU Method B.4 (Acute Toxicity: Dermal Irritation/Corrosion), oxazolidine was applied undiluted to the skin of rabbits for four hours and it was found to be corrosive. Application of diluted oxazolidine at a concentration of 5% resulted in slight skin irritation, and no effects were detected at a concentration of 1% (ECHA). [KI score =1].

Eyes

A study comparable to OECD guideline 405 was conducted using Grotan® OX, which contains para-formaldehyde and 2-HPA. Application of the undiluted product to the eyes of rabbits for 24 hours (unwashed) or 4 seconds (then washed) produced severe ocular reactions that were found to be irreversible. In short, when the neat substance is applied to the eyes of rabbits it is corrosive. Application of 0.2% Grotan® OX to the eyes of rabbits was found to be non-irritating (ECHA). [KI score=2].

E. Sensitisation

In a guinea pig maximization test conducted according to OECD Test Guideline 406, oxazolidine was identified as an extreme sensitizer. There is also supporting evidence from patch tests conducted in humans that indicate that this substance induces the highest frequency of contact allergy (ECHA). [KI score =2].

F. Repeated Dose Toxicity

Oral

As per OECD Test Guideline 408 (Repeated Dose 90-Day Oral Toxicity Study in Rodents), 10 male and 10 female rats were given oxazolidine via oral gavage once daily (7 days per week) for 90 days. The rats were administered the following doses: 0, 20, 60, 180, and 120 mg/kg bw (concentration 0, 0.4, 1.2, 3.6, and 2.4% in corn oil). At dose levels ≥60 mg/kg bw (LOAEL) and a concentration of ≥12 mg/mL, oxazolidine induced local effects in the stomach after repeated exposure via gavage. However, this finding is not relevant to humans. There were no effects observed at a daily dose of 20 mg/kg bw; therefore, a NOAEL was determined to be 20 mg/kg bw/day (ECHA) [KI score =1]).

As per OECD Test Guideline 408 (Repeated Dose 90 Day Oral Toxicity Study in Rodents), 10 male and 10 female rats were given oxazolidine via oral gavage once daily for 92 days in males and 93 days in female rats. The rats were administered the following doses: 0,30,72,180 mg/kg bw (concentration 0, 0.3, 0.72, or 1.8% in water). A LOAEL of 180 mg/kg bw/day was established based on effects on body weight, clinical chemistry, organ weights, and haematological and histological effects in the

high dose group of male rats. A NOAEL of 72 mg/kg bw/day was established based on changes in body weight, clinical chemistry and organ weights. The authors noted that this study has some lack of data interpretation and they noted that the results may have been influenced by an infection with mycoplasma pneumonia (ECHA) [KI score = 2].

Inhalation

There are no studies available.

Dermal

There are no studies available.

G. Genotoxicity

The test substance (hydrolysis products of oxazolidine) was not mutagenic in genotoxicity assays in the bone marrow of mice. This indicates that the substance is not genotoxic distant from the site of first contact. However, mutagenicity assays *in vitro* reveal the reactivity of the substance towards DNA, which corresponds to the reactivity of formaldehyde. Data on the hydrolysis product formaldehyde suggested more local than systemic mutagenic effects. Formaldehyde is genotoxic *in vitro,* and it induces local clastogenic effects *in vivo* (ECHA).

In Vitro Studies

Table 3 lists the *in vitro* genotoxicity studies on oxazolidine.

Table 3 In Vitro Genotoxicity Studies on Oxazolidine[1]

Test System	Results		Klimisch Score	Reference
	-S9	+S9		
Bacterial Reverse Mutation Assay (S.typhimurium TA 1535 TA 1537 TA98 TA 100 and E.coli WP2)	+	+	1	ECHA
Bacterial Reverse Mutation Assay (S.typhimurium TA 1535 TA 1537 T A98 TA 100 and TA 102)	-	-	2**	ECHA
Bacterial Reverse Mutation Assay (S.typhimurium TA 1535 TA 1537 TA 98 and TA 100))	-	-	2**	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	+	+	1	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	+	+	1	ECHA
Chromosomal aberrations (Chinese Hamster Lung)	+	+	1	ECHA

*+, positive; -, negative
** Ambiguous results, substance was not tested up to the cytotoxicity threshold
1 – Test substance was a mixture of para-formaldehyde and 2-HPA

In Vivo Studies

As per OECD Test Guideline 474 (Mammalian Erythrocyte Micronucleus Test) five male and five female mice were administered CONTRAM™ MBO (which contains para-formaldehyde and 2-HPA) via oral gavage for 24 hours at the following dose levels: 0, 30, 100, and 300 mg/kgbw (concentrations of 0,0.15, 0.5, and 1.5). The test substance was determined to be negative for genotoxicity given the fact that it did not induce a statistically significant increase in the number of micronuclei at a dose level up to 300 mg/kg bw. At the 300 mg/kg bw dose, slight to moderate reduced motility, slight ataxia, slight reduced muscle tone and slight dyspnoea was observed 15 minutes to 3 hours after administration of the test substance (ECHA). [Kl. Score = 2].

As per OECD Test Guideline 475 (Mammalian Bone Marrow Chromosome Aberration Test) five male and five female mice were administered Grotmar 71, which contains para-formaldehyde and 2-HPA, via oral gavage for two days at the following doses: 0, 92, 183, and 367 mg/kg bw (concentrations of :0.92, 1.83, and 3.67%). The test substance displayed no genotoxic effects at the conclusion of the study because it did not induce a statistically significant increase in chromosomal aberrations in the bone marrow of mice (ECHA).[KI score =2].

H. Carcinogenicity

There are no long-term carcinogenicity studies available on experimental animals for oxazolidine. However, this substance is assumed to hydrolyse rapidly within the body. There are probable carcinogenic effects related to the hydrolysis product formaldehyde. Formaldehyde has mutagenic activity *in vitro* but it does not induce systemic mutagenic *in vivo*. Formaldehyde does induce local mutagenic effects *in vivo*. Sufficient data are available on carcinogenicity of formaldehyde, as well as the mode of action. In experimental animals, formaldehyde induces tumours at the site of first contact, but it does not induce systemic carcinogenic effects. The results of epidemiological studies are conflicting. The local carcinogenic effects of formaldehyde are dependent on cytotoxicity and cell proliferation. At non-irritant concentrations tumour formation is not expected. Assuming that the possible mutagenic and carcinogenic effects of oxazolidine are based on the hydrolysis product formaldehyde, no carcinogenic effects are expected at these threshold concentrations (ECHA).

I. Reproductive and Developmental Toxicity

As per OECD Test Guideline 415 (One Generation Reproduction Toxicity Study before October 9, 2017), oxazolidine was administered at the following doses: 0, 5, 15, and 45 mg/kg bw/day once daily to 24 male and 24 female rats via oral gavage until day 20 postpartum. A general NOAEL for parental animals was determined to be 5 mg/kg bw/day based on histopathological effects in the forestomach of male rats administered 15 and 45 mg/kg of oxazolidine. A systemic NOAEL for parental animals was determined to be 15 mg/kg bw/day based on reduced body weights observed in the animals dosed with 45 mg/kg of oxazolidine. The NOAEL for reproduction/developmental toxicity was determined to be 15 mg/kg bw/day based on an increased incidence of post implantation and postnatal loss in the animals dosed with 45 mg/kg of oxazolidine. There were no effects noted in the F1 progeny during the weaning phase and at necropsy (ECHA). [KI score =1].

As per OECD Test Guideline 414 (Prenatal Developmental Toxicity Study), oxazolidine was administered via oral gavage to 24 pregnant rabbits at the following doses: 0,5, 45,90, and 135 mg/kg bw/day (concentration: 0, 0.25,2.25,4.5, and 6.75%) at gestation day 6-28. In the animals dosed with 135 mg/kg of oxazolidine, there was a decrease in body weight and increased mortality and abortions, which indicate maternal toxicity. At necropsy, local lesions were found in the stomach, and there was an increased incidence in dilation of the renal pelvis. There were no effects identified in the animals dosed with 90 mg/kg of oxazolidine, and the authors concluded that the effects identified in the stomach were due to the corn oil vehicle. Therefore, the authors determined that the NOAEL for maternal toxicity was 90 mg/kg bw/day (ECHA). [KI score =1].

There were no developmental effects detected at 90 mg/kg bw/day so the NOAEL for fetotoxicity was determined to be 90 mg/kg bw/day. At the high dose levels the number of early and late resorptions was increased, the number of foetuses decreased, and the post-implantation loss and mortality of foetuses during the 6-hour incubator stay increased. There was no increase in the incidence of retardations, variations, or malformations in any treatment group (ECHA). [KI score =1].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for oxazolidine follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

In a 90-day oral toxicity study, a NOAEL of 20 mg/kg bw/day was established based on local effects in the stomach. In a one generation reproductive toxicity study in rats, a systemic NOAEL for parental animals was determined to be 15 mg/kg bw/day based on reduced body weights observed in the animals dosed via oral gavage with 45 mg/kg of oxazolidine. The NOAEL for reproduction/ developmental toxicity was determined to be 15 mg/kg bw/day based on an increased incidence of post-implantation and postnatal loss in the animals dosed via oral gavage with 45 mg/kg of oxazolidine. The NOAEL of 15 mg/kg bw/day will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 15/(10 x 10 x 1 x 10 x 1) = 15/1000 = 0.015 mg/kg bw/day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.015 x 70 x 0.1)/2 = 0.0525 mg/L

Cancer

There were no carcinogenicity studies conducted on oxazolidine. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Oxazolidine does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Overall, oxazolidine is moderately toxic to aquatic life. The acute toxicity of oxazolidine is of low concern to fish and invertebrates and of moderate concern to algae. The chronic toxicity of oxazolidine is of moderate concern to invertebrates and algae. Based on hazard data, invertebrates are slightly more sensitive than algae in chronic toxicity studies.

B. Aquatic Toxicity

In aqueous media, oxazolidine is rapidly hydrolysed (DT_{50} < 1 hour). At a concentration of 0.0025% (equally to 25 mg/L) the hydrolysis equilibrium is nearly complete at the hydrolysis products formaldehyde and 2-HPA. Therefore, in the concentration range applied in ecotoxicity tests, the reaction product is completely or nearly completely hydrolysed, and thus, observed effects are caused by the hydrolysis products. The comparison of aquatic toxicity data for the substance and its hydrolysis products reveals clearly that the toxicity of the substance is exclusively determined by its formaldehyde content (ECHA).

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on oxazolidine.

Table 4: Acute Aquatic Toxicity Studies on Oxazolidine

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Danio rerio (Zebrafish)	96-hr LC_{50}	71	1	ECHA
Danio rerio (Zebrafish))	96-hr LC_{50}	57.7	1	ECHA
Daphnia magna	48-hr EC_{50}	29	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50}	5.7 (growth rate) 2.6 (biomass)	2	ECHA

Chronic Studies

There are no chronic studies on fish available. However, the available data on acute toxicity indicate that fish is the trophic level with the lowest sensitivity (ECHA).

As per OECD Test Guideline 211 (Daphnia magna Reproduction Test), *Daphnia magna* were exposed to oxazolidine for 21 days at concentrations ranging from 0.512 to 20.0 mg/L. Oxazolidine was found to be harmful toward daphnids reproduction and resulting 21-day no observed effect concentration (NOEC) was determined to be 1.3 mg/L based on mortality (ECHA). [KI score =1].

As per OECD Test Guideline 201 (Alga, Growth Inhibition Test) and EU Method C.3 (Algal Inhibition test), *Desmodesmus subspicatus* were exposed to oxazolidine for 72 hours at the following concentrations: 1.0, 2.2, 4.84, 10.65, and 23.43 mg/L. Oxazolidine was found to be harmful towards algae at low concentrations. The resulting 72-hour NOEC was determined to be 2.2 mg/L (growth rate) (ECHA).[KI score =2].

C. Terrestrial Toxicity

There are no studies available.

Furthermore, a K_{OC} value of 1 L/kg had been estimated for oxazolidine on the basis of a measured value log K_{OW} value for 5-methyl-oxazolidine. This value indicates a weak adsorption potential of the compound to soil and sediments (ECHA).

D. Calculation of PNEC

The PNEC calculations for oxazolidine follow the methodology discussed by DEWHA (2009).

PNEC Water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (57.7 mg/L), invertebrates (29 mg/L) and algae (5.7 mg/L). Results from chronic studies are available

for invertebrates (1.3 mg/L) and algae (2.2 mg/L). On the basis that the data consists of short-term studies for three trophic levels and long-term results studies for two trophic levels, an assessment factor of 50 has been applied to the lowest reported NOEC of 1.3 mg/L for invertebrates. The $PNEC_{water}$ is 0.026 mg/L.

PNEC Sediment

There are no toxicity data for sediment-dwelling organisms. Moreover, the substance is not expected to substantially partition to sediments. Nonetheless, a $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.017 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 0.819/1280 \times 1000 \times 0.026$
$= 0.017$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = 0.026 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 0.04)/1000 \times 2400]$
$= 8.19E\text{-}01\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 1 \times 0.04$
$= 0.04$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for oxazolidine based on OECD Test Guideline 121 is ≤1 L/kg (ECHA) [KI score =1].
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC Soil

There are no toxicity data for terrestrial or soil organisms. Moreover, the substance is not expected to strongly adsorb to soil. Nonetheless, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.00035 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (0.02/1500) \times 1000 \times 0.026$
$= 0.00035$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 kg/m^3 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 1 \times 0.02$
$= 0.02\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for oxazolidine based on OECD Test Guideline is 1 L/kg (ECHA) [KI score =1].
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

Oxazolidine is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on estimated BCF values of 1.41 L/kg for fish, oxazolidine does not meet the screening criteria for bioaccumulation.

The lowest chronic NOEC for oxazolidine is >0.1 mg/L. The acute $E(L)C_{50}$ values are >1 mg/L. Thus, oxazolidine does not meet the screening criteria for toxicity.

The overall conclusion is that oxazolidine is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for oxazolidine.

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9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on Relevant Databases?	Identified as Polymer of Low Concern	P criteria Fulfilled?	Other P Concerns	B Criteria Fulfilled?	T Criteria Fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Oxazolidine	66204-44-2	Not a PBT	No	No	No	No	No	No	1 (fish, inv) 2 (algae)	1	2

1 - PBT Assessment based on PBT Framework.
2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).
3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.
B = bioaccumulative
COC = constituent of concern
NA = not applicable
P = persistent
PBT = Persistent, Bioaccumulative and Toxic
T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
BCF	Bioconcentration factor
bw	body weight
CAS No.	Chemical Abstract Services Registry Number
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DoEE	Department of the Environment and Energy
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
HHRA	enHealth Human Risk Assessment
HPA	2-hydroxylpropylamine
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
Kl	Klimisch scoring system
K_{oc}	organic carbon normalised distribution coefficient
K_{ow}	octanol-water partition coefficient
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/kg bw/day	milligrams per kilogram body weight per day
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
OECD	Organization for Economic and Cooperation and Development

Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure-activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
UVCB	Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
Oxazolidine	66204-44-2	5.00E+01	1.50E+01	5.00E+00	1.25E+00	5.00E-02	1.25E-02	1.00E-03	2.50E-04	2.60E-02

**Concentration based on typical biocide dosing rates*

Notes:

mg/L = milligrams per liter

CAS = Chemical Abstracts Service

NA = not applicable

PNEC = predicted no effects concentration

RO = reverse osmosis

WMF = Water Management Facility

Qualitative Tier 2 Assessment

PolyDADMAC

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Cationic polymers are a component in a Water Management Facility (WMF) product used as a coagulant during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Cationic Polymer[a]	n/a	Polymer / coagulant	2 x 1000 L (IBC)
Aluminium Hydroxychloride	1327-41-9		
Water	7732-18-5		

[a] Identity unknown. Read-across to polydiallyldimethylammonium chloride [polyDADMAC (CAS No. 26062-79-3)].
CAS No = Chemical Abstracts Service Number
IBC = intermediate bulk container
L = litre
n/a = not available

As noted above and detailed in the SDS, the identity of the cationic polymer in the vendor product is unknown. Therefore, a read-across to polyDADMAC (CAS RN 26062-79-3)[2] was conducted for this assessment. Information compiled for polyDADMAC is provided in the risk assessment dossier included as **Attachment 2**. Results of the screening assessment are included in the dossier.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

[2] CAS RN - Chemical Abstracts Service Registry Number

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in **Attachment 2**. PolyDADMAC is not a carcinogen, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Cationic polymer[a]	6-month rat dietary study	None	2,000	600	3.3	12

[a] Identity unknown. Read-across to polydiallyldimethylammonium chloride [polyDADMAC] (CAS No. 26062-79-3).
CAS = Chemical Abstracts Service
mg/L = milligrams per litre
mg/kg-day = milligrams per litre-day
NOAEL = No observed adverse effect level
Refer to **Attachment 2** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water

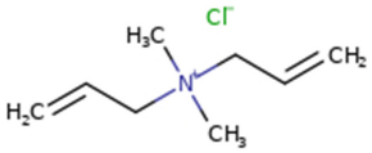
Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Cationic polymer[a]	Acute fish	6.5	50	0.13

[a] Identity unknown. Read-across to polydiallyldimethylammonium chloride polyDADMAC (CAS No. 26062-79-3).
EC_{50} = effects concentration – 50%
mg/L = milligrams per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

PolyDADMAC is a highly charged cationic homopolymer with high molecular weights; those used in water treatment may have molecular weights less than 500,000 daltons (Lyons and Vasconcellos, 1997). The molecular structure of polyDADMAC is presented in **Figure 1**.



(monomer shown)

Figure 1 Molecular Structure of PolyDADMAC[3]

Synthetic polymers are persistent in the environment. They are expected to be poorly biodegraded, and adsorption would be expected to be the primary process that determines its ecological concentrations and mobility (Lyons and Vasconcellos, 1997). As a cationic polymer, polyDADMAC will rapidly react with many kinds of naturally occurring substances, such as humic acids, lignins, silts, and clays (Lyons and Vasconcellos, 1997). Due to its physical properties (i.e., molecular size and partitioning behaviour), polyDADMAC is not expected to bioaccumulate.

The PBT assessment for polyDADMAC is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that polyDADMAC is not a PBT substance.

Human Health Hazards

There is a low concern for human health hazards. PolyDADMAC is not acutely toxic to humans by the oral route (LD_{50} > 5,000 mg/kg bw)[4]. Likewise, there are no adverse effects observed from repeated exposures through ingestion (lowest observed adverse effect level [LOAEL] of 1,000 milligrams per kilogram per day [mg/kg-day], a no observed adverse effect level [NOAEL] was not established).

Based on a review of repeated dose toxicity studies, TRVs were derived for polyDADMAC. The drinking water guideline value derived using the non-carcinogenic oral RfD is 12 mg/L (see **Table 2**). A detailed discussion of the drinking water guideline values is presented in **Attachment 2**.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents. Based on the treatment process described in **Attachment 1**, the cationic polymers would be bound to the solids present in the oily water and removed during clarification. As a result, this chemical would not be present in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

[3] Source https://chem.nlm.nih.gov/chemidplus/rn/26062-79-3

[4] LD50 = lethal dose of 50 percent of population; mg/kg bw – milligrams per kilogram body weight

PolyDADMAC is listed in Attachment B (Substances Considered Not To Require Control By Scheduling) of the *Standard for the Uniform Scheduling of Medicines and Poisons* (SUSMP) (Therapeutic Goods Administration [TGA], 2014). The reason given for the listing in Attachment B is 'Low Toxicity' and the area of use of the chemical is 'Water treatment' (NICNAS, 2017a). NICNAS identified polyDADMAC as a low concern for workers and the public under the operational scenarios assessed. Best practice chemical management was recommended to minimise worker and public exposure (NICNAS, 2017a).

Environmental Hazards

In standard acute aquatic toxicity tests, polyDADMAC, as a highly charged cationic polymer, is very toxic to aquatic life. PolyDADMAC will dissociate into polyammonium cations and chloride anions in the aquatic environment. Chloride ions are an essential constituent of electrolytes in all biological fluids responsible for maintaining acid/base balance, transmitting nerve impulses and regulating fluid in and out of cells (NCBI, 2015). The concentration of chloride ions is naturally regulated within organisms. Therefore, the toxicity of cationic polymers to fish is from the binding of the polyammonium cations in the polymer to the gill tissue, disrupting gill structure and function. Physical damage to fish gill by cationic polymers has been shown by Beisinger and Stokes (1986).

However, under environmental conditions, the toxicity of these polymers is mitigated by the presence of dissolved organic carbon (DOC) and suspended solids. Cationic polymers react with DOC in environmental waters to form insoluble complexes, which settle out of water and therefore are not bioavailable to cause toxic effects. It has previously been established that a reduction in likely toxicity by a factor of 110 is appropriate to apply to laboratory test results for cationic polymers with a high charge density to account for the mitigating effects of DOC on toxicity in natural environmental waters (Boethling and Nabholz, 1997).

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with the following Matters of National Environmental Significance [MNES] receptors:

- White-throated Snapping Turtle (*Elseya albagula*) – Critically endangered; and
- Fitzroy River Turtle (*Rheodytes leukops*) – Vulnerable.

These findings are consistent with an assessment completed by NICNAS in 2017. Based on an assessment of environmental hazards, NICNAS identified polyDADMAC as a chemical of low concern to the environment (NICNAS, 2017b). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

References

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TGA. (2014). Standard for the Uniform Scheduling of Medicines and Poisons.

Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration	
MAK MFC1 (multi floc coagulant)	Cationic Polymer Aluminium Hydroxychloride Water	n/a 1327-41-9 7732-18-5	20-40% 40-60% 20-60%	MAK MFC1	MAK Water Industrial	Oily Water Treatment Plant	1000L IBC		2 x 1000L (IBC)		0.8mg/L (AVG)		

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Purpose / Function	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration
					(mg/L)	Permeate notes	(mg/kg)	mg/kg	(mg/L)
MAK MFC1 (multi floc coagulant)	Cationic Polymer	n/a	polymer / coagulant	Removed with oily water sludge (solid waste)	NA	Oily water is clarified to remove solids and oils then run through the RO system. The amount relative to flux of RO system is <1%. Therefore, the net on permeate quality is deminimis. Therefore, no concentration of chemical in this product in the permeate.	NA	NA	NA
	Aluminium Hydroxychloride	1327-41-9			NA	Oily water is clarified to remove solids and oils then run through the RO system. The amount relative to flux of RO system is <1%. Therefore, the net on permeate quality is deminimis. Therefore, no concentration of chemical in this product in the permeate.	NA	NA	NA
	Water	7732-18-5			NA		NA	NA	NA

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Notes
MAK MFC1 (multi floc coagulant)	Cationic Polymer	n/a	The oily water is clarified to seperate solids and oils; then run through the RO system. Estimate 5% residual in brine, the balance is sludge.
	Aluminium Hydroxychloride	1327-41-9	The oily water is clarified to seperate solids and oils; then run through the RO system. Estimate 5% residual in brine, the balance is sludge. Estimate that chemical will dissociate to aluminium (Al) and Cl- at 40% Al and 55% Cl-.
	Water	7732-18-5	

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

POLYDADMAC
[POLYDIALLYLDIMETHYLAMMONIUM CHLORIDE]

This dossier on polyDADMAC presents the most critical studies pertinent to the risk assessment of polyDADMAC in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – PolyDADMAC was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. PolyDADMAC was assessed as a tier 2 chemical for acute and chronic toxicity. Therefore, polyDADMAC is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1. BACKGROUND

Polydiallyldimethylammonium chloride (polyDADMAC) are highly charged cationic polymers with high molecular weights. They are expected to be poorly biodegraded, and adsorption would be expected to be the primary process that determines its ecological concentrations and mobility. As a cationic polymer, polyDADMAC will rapidly react with many kinds of naturally occurring substances, such as humic acids, lignins, silts and clays. Due to its physical properties (i.e., molecular size), polyDADMAC is not expected to bioaccumulate. PolyDADMAC is not acutely toxic to humans by the oral route; nor does it exhibit any systemic toxicity from repeated exposures through ingestion. PolyDADMAC exhibits a moderate toxicity concern to aquatic organisms. The toxicity of these polymers is mitigated by the presence of dissolved organic carbon (DOC) and suspended solids. Cationic polymers react with DOC in environmental waters to form insoluble complexes, which settle out of water and therefore are not bioavailable to cause toxic effects.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Polydiallyldimethylammonium chloride
CAS RN: 26062-79-3
Molecular formula: $(C_8H_{16}N.Cl)_x$-
Molecular weight: Variable

Synonyms: PolyDADMAC; 2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer; Poly-2-propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride; N-N-dimethyl-N-2-propenyl-2-propen-1-aminium chloride, homopolymer; poly-N,N-dimethyl-N-N-diallyammonium chloride; polyquaternium-6

3. PHYSICO-CHEMICAL PROPERTIES

PolyDADMAC are highly charged cationic homopolymers with high molecular weights; those used in water treatment may have molecular weights less than 500,000 daltons (Lyons and Vasconcellos, 1997).

Limited information is available on the physico-chemical properties of polyDADMAC. The information contained in Table 1 is based on diallyldimethylammonium chloride (DADMAC) (CAS No. 7398-69-8). PolyDADMAC is a homopolymer of DADMAC.

Table 1 Overview of the Physico-chemical Properties of DADMAC

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	-	ECHA
Melting Point/Freezing Point	-25 °C @ 101.3 kPa	1	ECHA
Boiling Point	118 °C @ 101.3 kPa	1	ECHA
Density	1,030 – 1,050 kg/m^3 @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	Estimated to be -2.49 @ 20°C using KOWWIN	2	ECHA
Water Solubility	Estimated to be 1,000 g/L @ 25°C	2	ECHA

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. PolyDADMAC is also listed in Appendix B (Substances Considered Not To Require Control By Scheduling) of the *Standard for the Uniform Scheduling of Medicines and Poisons* (SUSMP) (Therapeutic Goods Administration [TGA], 2014). The reason given for listing in Appendix B is 'Low Toxicity' and the area of use of the chemical is 'Water treatment' (NICNAS, 2017a). No other specific environmental regulatory controls or concerns were identified within Australia and internationally for polyDADMAC.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5. ENVIRONMENTAL FATE SUMMARY

A. Summary

PolyDADMAC are highly charged cationic polymers with high molecular weights. They are expected to be poorly biodegraded, and adsorption would be expected to be the primary process that determines its ecological concentrations and mobility (Lyons and Vasconcellos, 1997). As a cationic polymer, polyDADMAC will rapidly react with many kinds of naturally occurring substances, such as humic acids, lignins, silts and clays (Lyons and Vasconcellos, 1997).

PolyDADMAC will dissociate into polyammonium cations and chloride anions in the aquatic environment. Chloride ions are an essential constituent of electrolytes in all biological fluids responsible for maintaining acid/base balance, transmitting nerve impulses and regulating fluid in and out of cells (NCBI, 2015). The concentration of chloride ions is naturally regulated within organisms. Therefore, consistent with NICNAS (NICNAS, 2017b), this discussion is focused on the environmental fate and effects of the synthetic polyammonium cations.

B. Biodegradation

Due to its physical properties (i.e., molecular size), polyDADMAC is expected to be poorly degraded. This finding is consistent with DADMAC which is not readily biodegradable according to the OECD criteria (ECHA). [Kl. score = 1]

C. Bioaccumulation

Due to its physical properties (*i.e.*, molecular size), polyDADMAC is not expected to bioaccumulate.

6. HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

PolyDADMAC is not acutely toxic by the oral route; nor does it exhibit any systemic toxicity from repeated exposures through ingestion.

B. Acute Toxicity

There were no deaths in rats given a single oral dose of 5,000 mg/kg polyDADMAC. The oral LD50 in rats is >5,000 mg/kg (USEPA, 2016a).

C. Irritation

No studies were located.

D. Sensitisation

No studies were located.

E. Repeated Dose Toxicity

<u>Oral</u>

Male and female Sprague Dawley (SD) rats were fed in their diet 0, 1,000 or 2,000 mg/kg polyDADMAC for six months. There were no clinical signs of toxicity. Two low-dose males were sacrificed in a moribund condition, while one low-dose male and one high-dose male died during the exposure period. Feed consumption was significantly increased in the treated groups compared to controls. Body weight gain was significantly lower in the treated animals compared to the controls. Final body weights were significantly lower in all dose groups compared to controls (10.4% and 19.5% in males; 6.6% and 10% in females for the low- and high-dose groups, respectively). Hematology and clinical chemistry parameters and urinalysis showed no biologically significant differences between treated and control groups. Relative liver weights were decreased in the >1,000

mg/kg males and 2,000 mg/kg females. Relative heart weights were decreased in the 2,000 mg/kg (both sexes), and relative kidney weights were decreased in the 2,000 mg/kg males. The histopathologic examination showed no treatment-related changes in these organs. No other compound-related pathology was observed, although histopathologic effects were seen in the lungs and urinary tract in animals of all groups. The LOAEL for this study is 1,000 mg/kg-day based on reduced body weights and body weight gain; a NOAEL was not established (USEPA, 2016b).

Inhalation

No studies were located.

Dermal

No studies were located.

F. Genotoxicity

No studies were located.

G. Carcinogenicity

No studies were located.

H. Reproductive Developmental Toxicity

No studies were located.

I. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for polyDADMAC follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

PolyDADMAC was tested in a six-month rat feeding study. No target organs were identified, and a NOAEL was not established. The LOAEL was 1,000 mg/kg-day based on reduced body weights and body weight gain. It is unclear from the limited data whether these changes in the treated animals are due to a direct or indirect effect of polyDADMAC. PolyDADMAC has a high molecular weight and would not be expected to be absorbed from the gastrointestinal tract. Feed consumption was significantly increased in the treated rats (both dose groups) even though body weights and body weight gain were reduced. A likely explanation for these findings is that the weight changes and feed consumption reflect the nutritional status of the treated animals due to the bulk presence of high levels of polymer in the feed and not to systemic toxicity. Given the absence of any other effects, it is proposed that the NOAEL for systemic toxicity in this study is 2,000 mg/kg-day, the highest dose tested.

The NOAEL of 2,000 mg/kg-day will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 2

Oral RfD = 2,000/(10 x 10 x 1 x 3 x 2) = 2,000/600 = 3.3 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (3.3 x 70 x 0.1)/2 = 12 mg/L

Cancer

No carcinogenicity studies were located; thus, a cancer reference value was not derived.

J. Human Health Hazard Assessment of Physico-Chemical Properties

PolyDADMAC does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

PolyDADMAC exhibits a moderate toxicity concern to aquatic organisms. However, under environmental conditions, the toxicity of these polymers is mitigated by the presence of DOC and suspended solids. Cationic polymers react with DOC in environmental waters to form insoluble complexes, which settle out of water and therefore are not bioavailable to cause toxic effects. It has previously been established that a reduction in likely toxicity by a factor of 110 is appropriate to apply to laboratory test results for cationic polymers with a high charge density to account for the mitigating effects of DOC on toxicity in natural environmental waters (Boethling and Nabholz, 1997).

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on polyDADMAC.

Table 3 Acute Aquatic Toxicity Studies on polyDADMAC

Test Species	Endpoint	Results (mg/L)	Reference
Bluegill	96-hour LC_{50}	0.9	USEPA, 2016c
Bluegill	96-hour LC_{50}	0.32	USEPA, 2016d
Rainbow trout	96-hour LC_{50}	0.32	USEPA, 2016d
Rainbow trout	96-hour LC_{50}	0.42	USEPA, 2016e
Rainbow trout	96-hour LC_{50}	0.77	USEPA, 2016f
Fathead minnow	96-hour LC_{50}	0.3	USEPA, 2016g
Fathead minnow	96-hour LC_{50}	6.51*	USEPA, 2016g
Fathead minnow	96-hour LC_{50}	0.46	Cary et al., (1987)
Fathead minnow	96-hour LC_{50}	6.5***	Cary et al., (1987)
Daphnia magna	48-hour EC_{50}	0.23	USEPA, 2016g
Daphnia magna	48-hour EC_{50}	11.8**	USEPA, 2016g
Daphnia magna	48-hour EC_{50}	0.33	USEPA, 2016h
Daphnia magna	48-hour EC_{50}	0.2	Cary et al., (1987)
Daphnia magna	48-hour EC_{50}	7.4***	Cary et al., (1987)

*10 mg/L humic acid in standard laboratory water.
**10 mg/L TOC in standard laboratory water.
***50 mg/L humic acid in standard laboratory water.

In standard acute aquatic toxicity tests, PolyDADMAC, as a highly charged cationic polymer, is very toxic to fish and *Daphnia magna*. The toxicity of cationic polymers to fish is from the binding of the polymer to gill tissue, disrupting gill structure and function. Physical damage to fish gill by cationic polymers has been shown by Biesinger and Stokes (1986).

The presence of dissolved organic carbon and suspended solids is known to significantly mitigate the toxicity of cationic polymers under typical environmental exposure conditions (Boethling and Nabholz, 1997). Table 3 also shows the change in acute toxicity when suspended solids or total organic carbon (TOC) is added to the standard laboratory water used in the toxicity tests. In the presence of humic acid or TOC, the EC_{50} values for fathead minnow and *Daphnia magna* increase by 21.7-fold and 51.3-fold, respectively. A similar effect of humic acid on the acute toxicity of polyDADMAC on fish and *Daphnia magna* was reported by Cary et al. (1987). The studies by Cary et al. (1987) also showed increases in varying amounts in the EC_{50} values for fathead minnow and *Daphnia magna* with bentonite, illite, kaolin, silica, tannic acid, lignin, lignosite and fulvic acid. The concentrations of suspended solids and DOC in the studies by Cary et al. (1987) were considered to be low estimates of levels found in the natural environments. These findings demonstrate that toxicity tests conducted on cationic polymers, such as polyDADMAC, using water with no organic carbon will likely overestimate the toxicity of these polymers in the environment.

Chronic Studies

No studies were located for polyDADMAC. The ratio of the acute toxicity to chronic toxicity for polyDADMAC is expected to be low. In 21-day *Daphnia magna* reproduction studies, three cationic polymers had 21-day threshold levels for survival that were higher by order of magnitude than the 48-hour TL_{50} values. The test solutions in these studies were renewed several times along with food, which served as new organic matter. The cationic polymer bioavailability was likely reduced from the adsorption to the food (Biesinger et al., 1976). In another study, low acute to chronic ratios was observed for a cationic polymer for *Ceriodaphnia dubia* and fathead minnows (Godwin-Saad et al., 1994).

It cannot be determined from the standard chronic tests if the adsorbed polymer is ingested or simply becomes unavailable by flocculating and/or settling. In any case, the low acute to chronic ratios of these cationic polymers appears to be best correlated with acute effects (Lyons and Vasconcellos, 1997).

C. Terrestrial Toxicity

No studies were located.

D. Calculation of PNEC

The PNEC calculations for polyDADMAC follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for two trophic levels. Acute EC_{50} values are available for fish (0.2 mg/L) and *Daphnia magna* (0.3 mg/L) in standard laboratory water; and for fish (6.5 mg/L) and *Daphnia magna* (11.8 mg/L) in standard laboratory water with the addition of humic acid or TOC. The PNEC water will be based on the EC_{50} values from the acute toxicity tests conducted with humic acid in the dilution water because this most likely represents the environmental conditions for which this assessment is being conducted. Furthermore, an assessment factor of 50 is proposed because chronic toxicity is expected to be similar to the acute toxicity of polyDADMAC (when tested in the presence of humic acid) because of the adsorption of the polymer to organic matter (food source) that would occur in standard test methods; hence, an assessment factor will be used for chronic

testing for two trophic levels. An assessment factor of 50 has been applied to the EC_{50} value of 6.5 mg/L for fish. The $PNEC_{water}$ is 0.13 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. The K_{ow} and K_{oc} have not been experimentally derived for polyDADMAC; these values cannot be estimated using QSAR models because of the high molecular weight of polyDADMAC. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$.

PNEC soil

There are no toxicity data for soil-dwelling organisms. The K_{ow} and K_{oc} have not been experimentally derived for polyDADMAC; these values cannot be estimated using QSAR models because of the high molecular weight of polyDADMAC. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{soil}$.

8. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

PolyDADMAC is a high molecular weight polymer; it is expected to be poorly biodegraded. Thus, it meets the screening criteria for persistence.

PolyDADMAC is a high molecular weight polymer that is not expected to be bioavailable to aquatic or terrestrial organisms. Thus, it is not expected to bioaccumulate.

No chronic aquatic toxicity studies have been conducted on polyDADMAC. The EC_{50} values of fish and *Daphnia magna* for acute toxicity tests conducted with humic acid or TOC in dilution water were >1 mg/L. Thus, polyDADMAC does not meet the screening criteria for toxicity.

The overall conclusion is that polyDADMAC is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for polyDADMAC.

9. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
PolyDADMAC	26062-79-3	Not a PBT	No	No	Yes	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

ADWG. (2011). National Water Quality Management Strategy. Australian Drinking Water Guidelines, Section 6, Australian Government, National Health and Medical Research Council, Natural Resource Management Ministerial Council.

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B. Abbreviations and Acronyms

ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
kg	kilogram
Kl	Klimisch scoring system
KOWWIN	USEPA program to estimate the organic carbon-normalized sorption coefficient for soil and sediment
kPa	kilopascal
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SD	Sprague Dawley

SGG	Synthetic Greenhouse Gases
SUSMP	Standard for the Uniform Scheduling of Medicines and Poisons
TGA	Therapeutic Good Administration
TL_{50}	time required for 50% of inoculated population to die
TOC	total organic carbon
USEPA	United States Environmental Protection Agency

Qualitative Tier 2 Assessment

Polyquaternium-33

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Cationic polymers are a component in a Water Management Facility (WMF) product used as a coagulant during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Adipic Acid Cationic acrylamide copolymer	124-04-9 69418-26-4	Sludge polymer	1000 kg

CAS No = Chemical Abstracts Service Number
kg = kilogram

The identity of the cationic polymer in the vendor product is acrylamide-acroloyloxyethyltrimethyl ammonium chloride (also known as polyquaternium-33) (CAS RN 69418-26-4)[2]. Information compiled for polyquaternium-33 is provided in the risk assessment dossier included as **Attachment 2**. Results of the screening assessment are included in the dossier.

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in **Attachment 2**. As detailed in the attachment and

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

[2] CAS RN - Chemical Abstracts Service Registry Number

presented in **Table 2**, no data are available to derive toxicological reference and drinking water guidance values for polyquaternium-33.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Polyquaternium-33 (69418-26-4)	- [a]	-	-	-	-	-

[a] – No data available.
CAS = Chemical Abstracts Service
mg/kg-day = milligrams per kilogram-day
mg/L = milligrams per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 2** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to the dossier provided in **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Polyquaternium-33 (69418-26-4)	Acute fish	1-10	1,000	0.001-0.01

EC_{50} = effects concentration – 50%
mg/L = milligrams per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

Polyquaternium-33 is a copolymer of trimethylaminoethylacetate salt and acrylamide. It is a highly charged cationic homopolymer with high molecular weights. While specific information is not available, typical flocculants that are cationic polyacrylamide-based copolymers have molecular weights that can range from 1 million to >50 million (Lyons and Vasconcellos, 1997). The molecular structure of polyquaternium-33 is presented in **Figure 1**.

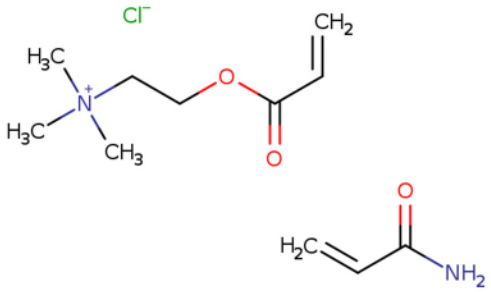

Figure 1 Molecular Structure of Polyquaternium-33[3]

Synthetic polymers are persistent in the environment. They are expected to be poorly biodegraded, and adsorption would be expected to be the primary process that determines its ecological concentrations and mobility (Lyons and Vasconcellos, 1997). As a cationic polymer, polyquaternium-33 will rapidly react with many kinds of naturally occurring substances, such as humic acids, lignins, silts and clays (Lyons and Vasconcellos, 1997). Due to its physical properties (i.e., molecular size), polyquaternium-33 is not expected to bioaccumulate.

The PBT assessment for polyquaternium-33 is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that polyquaternium-33 is not a PBT substance.

Human Health Hazards

There is a low concern for human health hazards. Polyquaternium-33 is not acutely toxic to humans by the oral route (LD_{50} > 5,000 mg/kg bw)[4]. Likewise, it is non-irritating to the skin and is not a skin sensitiser.

No data are available to derive toxicological reference and drinking water guideline values for polyquaternium-33. Additional discussion is included in the dossier provided in **Attachment 2**.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents. Based on the treatment process described in **Attachment 1**, the cationic polymers would be bound to the solids

[3] Source https://chem.nlm.nih.gov/chemidplus/rn/69418-26-4

[4] LD50 = lethal dose of 50 percent of population; mg/kg bw – milligrams per kilogram body weight

present in the oily water and removed during clarification. As a result, this chemical would not be present in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

In standard acute aquatic toxicity tests, polyquaternium-33, as a highly charged cationic polymer, has a moderate acute toxicity concern to aquatic organisms. However, under environmental conditions, the toxicity of these polymers is mitigated by the presence of dissolved organic carbon (DOC) and suspended solids. Cationic polymers react with DOC in environmental waters to form insoluble complexes, which settle out of water and therefore are not bioavailable to cause toxic effects. It has previously been established that a reduction in likely toxicity by a factor of 110 is appropriate to apply to laboratory test results for cationic polymers with a high charge density to account for the mitigating effects of DOC on toxicity in natural environmental waters (Boethling and Nabholz, 1997).

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with the following Matters of National Environmental Significance [MNES] receptors:

- White-throated Snapping Turtle (*Elseya albagula*) – Critically endangered; and
- Fitzroy River Turtle (*Rheodytes leukops*) – Vulnerable.

These findings are consistent with an assessment completed by NICNAS in 2017 for a similar cationic polymer (polyDADMAC). Based on an assessment of environmental hazards, NICNAS identified polyDADMAC as a chemical of low concern to the environment (NICNAS, 2017). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

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Lyons, L.A., and Vasconcellos, S.R. (1997). Water treatment polymers. In: Ecological Assessment of Polymers. Strategies for Product Stewardship and Regulatory Programs (Hamilton, J.D. and R. Sutcliffe, Eds.), pp. 113-145, Wiley.

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Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Hydrex 6926 (Sludge Polymer)	Adipic Acid Cationic acrylamide copolymer	124-04-9 69418-26-4	1-5% 80-90%	Hydrex 6926	Veolia Water Solutions	Reverse Osmosis Plant	25kg bags	100%	1000kg	100%	2mg/L (AVG)	100%	7300L	sludge polymer

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
L = litres
kg = kilograms
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration
				(mg/L)	Permeate notes	(mg/kg)	(mg/kg)	(mg/L)
Hydrex 6926 (Sludge Polymer)	Adipic Acid	124-04-9	Removed with Actiflo sludge (solid waste)	NA	This product is not directed to the permeate stream.	NA	NA	NA
	Cationic acrylamide copolymer	69418-26-4		NA	This product is not directed to the permeate stream.	NA	NA	NA

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
L = litres
kg = kilograms
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Notes
Hydrex 6926 (Sludge Polymer)	Adipic Acid	124-04-9	This product not directed to brine dams.
	Cationic acrylamide copolymer	69418-26-4	This product not directed to brine dams.

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
L = litres
kg = kilograms
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

ACRYLAMIDE, (2-ACRYLOYLOXYETHYLTRIMETHYLAMMONIUM CHLORIDE)

This dossier on acrylamide, (2-acryloyloxyethyltrimethylammonium chloride) (also known as polyquaternium-33) presents the most critical studies pertinent to the risk assessment of polyquaternium-33 in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Polyquaternium-33 was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Polyquaternium-33 was assessed as a tier 2 chemical for acute toxicity and as a tier 2 chemical for chronic toxicity. Therefore, polyquaternium-33 is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

Polyquaternium-33 is a copolymer of trimethylaminoethylacetate salt and acrylamide. Polyquaternium-33 is a highly charged cationic polymer with high molecular weights. It is used as flocculent, retention and drainage aid in the manufacture of food contact paper and paper board (FDA, 2013).

It is expected to be poorly biodegraded and adsorption would be expected to be the primary process that determines its ecological concentrations and mobility. As a cationic polymer, polyquaternium-33 will rapidly react with many kinds of naturally occurring substances, such as humic acids, lignins, silts and clays. Due to its physical properties (i.e. molecular size), polyquaternium-33 is not expected to bioaccumulate. The acute toxicity of polyquaternium-33 is very low by the oral route. It is non-irritating to the skin and is not a skin sensitiser. No other data are available regarding the human health hazard of polyquaternium-33. Polyquaternium-33 is a moderate acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): prop-2-enamide;trimethyl(2-prop-2-enoyloxyethyl)azanium; chloride
CAS RN: 69418-26-4
Molecular formula: $(C_8H_{16}ClNO_2)x.(C_3H_5NO)_x$
Molecular weight: No information is available. It is expected to be a high molecular weight polymer.

Synonyms: Acrylamide, (2-acryloyloxyethyl)trimethylammonium chloride polymer; ethanaminium, N,N,N,trimethyl-2-[1-oxo-2-propenyl)oxy]-, chloride, polymer with 2-propenamide; polyquaternium-33

3 PHYSICO-CHEMICAL PROPERTIES

The commercial polymer is a white to off-white powder. It is soluble in water, forming a viscous solution (BASF, 2010; WaterSolve, 2013).

While specific information is not available, typical flocculants that are cationic polyacrylamide-based copolymers have molecular weights that can range from 1 million to >50 million g/mol (Lyons and Vasconcellos, 1997).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 1). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for acrylamide, (2-acryloyloxyethyltrimethylammonium chloride).

Table 1 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Polyquaternium-33 is a highly charged cationic polymer with high molecular weights. It is expected to be poorly biodegraded and adsorption would be expected to be the primary process that determines its ecological concentrations and mobility (Lyons and Vasconcellos, 1997). As a cationic polymer, polyquaternium-33 will rapidly react with many kinds of naturally occurring substances, such as humic acids, lignins, silts and clays (Lyons and Vasconcellos, 1997).

Due to its physical properties (i.e. molecular size), polyquaternium-33 is not expected to bioaccumulate.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of polyquaternium-33 is very low by the oral route. It is non-irritating to the skin and is not a skin sensitiser. No other data are available regarding the human health hazard of polyquaternium-33.

B. Acute Toxicity

The oral LD_{50} in rats is >5,000 mg/kg (BASF, 2010; WaterSolve, 2013). [Kl. score = 4]

C. Irritation

Polyquaternium-33 is non-irritating to the skin of rabbits (BASF, 2010; WaterSolve, 2013). [Kl. score = 4]

No eye irritation studies are available. Polyquaternium-33 is expected to be a non-irritant to the eyes of rabbits (BASF, 2010; WaterSolve, 2013).

D. Sensitisation

Polyquaternium-33 is not a skin sensitiser to guinea pigs (WaterSolve, 2013).

E. Repeated Dose Toxicity

No studies are available.

F. Genotoxicity

No studies are available.

G. Carcinogenicity

No studies are available.

H. Reproductive Toxicity

No studies are available.

I. Developmental Toxicity

No studies are available.

J. Derivation Of Toxicological Reference And Drinking Water Guidance Values

No data are available to derive toxicological reference and drinking water guidance values for polyquaternium-33.

K. HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

Polyquaternium-33 does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Polyquaternium-33 has a moderate acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

The 96-hour LC_{50} to fish was reported to be 1 – 10 mg/L (BASF, 2010; WaterSolve, 2013). [Kl. score = 4]

The 48-hour EC_{50} to *Daphnia magna* was approximately 35 mg/L (WaterSolve, 2013). [Kl. score = 4]

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for polyquaternium-33 follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for two trophic levels. Acute EC_{50} values are available for fish (1-10 mg/L) and invertebrates (35 mg/L). On the basis that the data consist of short-term results from two trophic levels, an assessment factor of 1,000 has been applied to the lowest EC_{50} value of 1-10 mg/L for fish. The $PNEC_{water}$ is 0.001-0.01 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. The K_{ow} and K_{oc} have not been experimentally derived for polyquaternium-33; these values cannot be estimated using QSAR models because of the high molecular weight of polyquaternium-33. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$.

PNEC soil

There are no toxicity data for soil-dwelling organisms. The K_{ow} and K_{oc} have not been experimentally derived for polyquaternium-33; these values cannot be estimated using QSAR models because of the high molecular weight of polyquaternium-33. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{soil}$.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Polyquaternium-33 is a large molecular weight, water-soluble polymer. It is not expected to be readily biodegradable; thus, it meets the screening criteria for persistence.

Polyquaternium-33 is not expected to be bioavailable to aquatic or terrestrial organisms because of its large molecular weight and size. Thus, it is not expected to meet the criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on polyquaternium-33. The EC_{50} values from the acute aquatic toxicity studies on polyquaternium-33 are >1 mg/L. Thus, it is does not meet the screening criteria for toxicity.

The overall conclusion is that polyquaternium-33 is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for polyquaternium-33.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Polyquaternium-33	69418-26-4	Not a PBT	No	No	Yes[a]	No	No	No	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

[a] – high molecular weight polymer

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
LC	lethal concentration

LD	lethal dose
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases

Qualitative Tier 2 Assessment

Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl)

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterised by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3 kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl) is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to enhance the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl)	68155-20-4	surfactant	0.00051%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

While no specific composition data are available on amides, tall oils fatty, N,N-bis(hydroxyethyl), it is expected to be a mixture of diethanolamides of the fatty acids that constitute tall oil, which is composed of predominantly C18 unsaturated fatty acids: 48% oleic acid, 35% linoleic acid, 7% conjugated linoleic acid.

As there are no available studies on amides, tall oils fatty, N,N-bis(hydroxyethyl), this assessment is based on information on amides, C18-unsatd, N,N-bis(hydroxyethyl) [CAS No. 93-83-4] (also known as oleamide DEA. This is justified because amides, tall oils fatty, N,N-bis(hydroxyethyl) is

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

predominantly diethanolamides of unsaturated C18 fatty acids similar to the composition of oleamide DEA.

The assessment of toxicity of oleamide DEA was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. Oleamide DEA is not carcinogenic, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl) (68155-20-4)[a]	OECD 407	None observed	750	1000	0.75	2.63

[a]Information not available. Read-across to oleamide DEA (CAS No. 93-83-4).
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil.

The determination of TRVs was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl) (68155-20-4)[a]	Chronic *Daphnia*	0.07	10	0.007

[a]Information not available. Read-across to oleamide DEA (CAS No. 93-83-4).
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration

PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 3 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl) (68155-20-4)[a]	[b]	-	-	0.18

[a]Information not available. Read-across to oleamide DEA (CAS No. 93-83-4).
[b]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Amides, Tall Oils Fatty, N,N-Bis(Hydroxyethyl) (68155-20-4)[a]	[b]	-	-	0.16

[a]Information not available. Read-across to oleamide DEA (CAS No. 93-83-4).
[b]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

While no specific composition data are available on amides, tall oils fatty, N,N-bis(hydroxyethyl), it is expected to be a mixture of diethanolamides of the fatty acids that constitute tall oil, which is composed of predominantly C18 unsaturated fatty acids: 48% oleic acid, 35% linoleic acid, 7% conjugated linoleic acid.

As there are no available studies on amides, tall oils fatty, N,N-bis(hydroxyethyl), as previously noted this assessment is based on information on oleamide DEA [CAS No. 93-83-4]. This is justified because amides, tall oils fatty, N,N-bis(hydroxyethyl) is predominantly diethanolamides of unsaturated C18 fatty acids similar to the composition of oleamide DEA.

Oleamide DEA is produced by the condensation of oleic acid and diethanolamine. It is a substance of unknown or variable composition, complex reaction products or biological materials (UVCB). The molecular structure of oleamide DEA is presented in **Figure 1**.

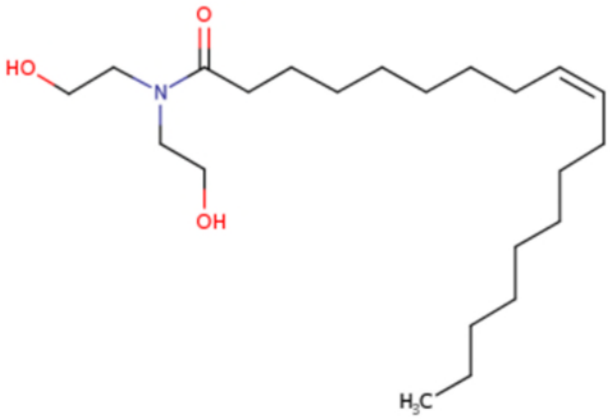

Figure 1 Molecular Structure of oleamide DEA [2]

Like other fatty acid diethanolamides, oleamide DEA is widely used in cosmetics as an emollient, thickener, and foam stabilizer and is present in approximately 121 cosmetic formulations of bath additives, shampoos, conditioners, lipsticks, and hair dyes. In these formulations, the concentration of diethanolamide ranges from 0.1% to 25% (NTP, 1999). Other applications include use as a surfactant in bar soaps, light-duty detergents, and dishwashing detergents (CTFA, 1985).

Oleamide DEA is readily biodegradable, has a moderate potential to sorb to sediments and soil, and a low potential to bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for oleamide DEA is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that oleamide DEA is not a PBT substance.

Human Health Hazards

The acute toxicity of oleamide DEA is low by the oral and dermal routes. It is a skin and eye irritant. It is not considered a skin sensitiser.

Repeated dose toxicity studies by the oral route did not show adverse effects; studies conducted by the dermal route showed irritation at the site of contact and systemic toxicity. Oleamide DEA is not a developmental toxicant. It is not genotoxic. Lifetime dermal studies on oleamide DEA showed no carcinogenic effects in rats or mice.

Based on a review of repeated dose and developmental toxicity studies, a TRV was derived for oleamide DEA. The drinking water guideline value derived using the non-carcinogenic oral RfD is 2.63 milligrams per litre (mg/L) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

[2] Source https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID8026563

Oleamide DEA may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to oleamide DEA in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, oleamide DEA is readily biodegradable and does not persist in the environment. In an OECD 301 D test, degradation was 70% after 28 days.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard acute aquatic toxicity tests, oleamide DEA is moderately toxic to fish and invertebrates, but slightly toxic to algae. Chronic toxicity towards fish and aquatic invertebrates is of the same order of magnitude. However, algae (*Desmodesmus subspicatus)* were somewhat less sensitive (ECHA). Terrestrial studies are not available.

Oleamide DEA is readily biodegradable and therefore is not persistent in the environment. It does not bioaccumulate.

PNECs for oleamide DEA are provided in **Tables 3 – 5**. Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs in water. There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released produced water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of oleamide DEA in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, first, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The concentration of oleamide DEA within the stimulation fluids will decrease in response to biodegradation and photolytic degradation of constituents over time. Chemical-specific biodegradation information presented in the dossier was used for the assessment.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system.

Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

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Attachment 1 Risk Assessment Dossier

AMIDES, TALL OILS FATTY, N,N-BIS(HYDROXYETHYL)

This dossier on amides, tall oils fatty, N,N-bis(hydroxyethyl) presents the most critical studies pertinent to the risk assessment of amides, tall oils fatty, N,N-bis(hydroxyethyl) in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997; Kl).

Screening Assessment Conclusion – Amides, tall oils fatty, N,N-bis(hydroxyethyl) was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Amides, tall oils fatty, N,N-bis(hydroxyethyl)was assessed as a tier 2 chemical for acute and chronic toxicity. Therefore, Amides, tall oils fatty, N,N-bis(hydroxyethyl)is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1. BACKGROUND

While no specific composition data are available on amides, tall oils fatty, N,N-bis(hydroxyethyl), it is expected to be a mixture of diethanolamides of the fatty acids that constitute tall oil, which is composed of predominantly C18 unsaturated fatty acids: 48% oleic acid, 35% linoleic acid, 7% conjugated linoleic acid.

As there are no available studies on CAS 68155-20-4, this dossier is based on information on amides, C18-unsatd, N,N-bis(hydroxyethyl) [CAS No. 93-83-4]. This is justified because amides, tall oils fatty, N,N-bis(hydroxyethyl) is predominantly diethanolamides of unsaturated C18 fatty acids similar to the composition of the target substance CAS 68155-20-4.

Amides, C18-unsatd, N,N-bis(hydroxyethyl) (also known as oleamide DEA) are readily biodegradable, have a moderate potential to sorb to sediments and soil, and a low potential to bioaccumulate. The acute toxicity of oleamide DEA is low by the oral and dermal routes. It is a skin and eye irritant. However, it is not considered a skin sensitiser. It is not toxic via repeated doses; has no reported reproductive or developmental effects; and, is not considered genotoxic or carcinogenic. It has a moderate toxicity to aquatic organisms.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Amides, tall oils fatty, N,N-bis(hydroxyethyl)

CAS RN: 68155-20-4

Synonyms: N,N-bis(2-hydroxyethyl)tall oil acid amide; N,N-bis(2-hydroxyethyl)tall oil fatty amides; Diethanolamine tall oil acid amide; tall oil acid diethanolamide; tallamide DEA; tall oil fatty acid diethanolamide; tall oil fatty acids, diethanolamide; tall oil fatty acids, diethanolamide condensate; tall oil fatty acids, diethanolamine amide

AMIDES, C18-UNSATURATED, N,N-BIS(HYDROXYETHYL)

Chemical Name (IUPAC): Oleamide DEA
CAS RN: 93-83-4
Molecular formula: $C_{22}H_{43}NO_3$ (UVCB substance)
Molecular weight: 369.6 g/mol (UVCB substance)

Synonyms: Oleyl diethanolamide;(9Z)-N,N-Bis(2-hydroxyethyl)-9-octadecenamide; (z)-n,n-bis(2-hydroxyethyl)-9-octadecenamide; 9-Octadecenamide, N,N-bis(2-hydroxyethyl)-, (Z)-; Alkamide DO-280;N,N-Bis(2-hydroxyethyl)-9-octadecenamide; Alrosol O; Amisol ode; Clindrol 2000; Clindrol 2020, Comperlan OD; Diethanololeamide; EMID 6545; Emulsifier WHC; Lauridit OD; Mackamide O, Marlamid D 1885, N,N-Diethanololeamide, Nitrene NO, Oleamide, N,N-bis(2-hydroxyethyl)-, Oleic acid diethanolamide, Oleic acid diethanolamine condensate, Oleic diethanolamide, Schercomid ODA, Stafoam DO, Steinamid DO 280SE, Witcamide 511C

3. PHYSICO-CHEMICAL PROPERTIES

No information is available on amides, tall oils fatty, N,N-bis(hydroxyethyl). Key physical and chemical properties for the surrogate substance (oleamide DEA) are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Oleamide DEA [CAS No. 93-83-4]

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Liquid	2	ECHA
Melting point	Approximately -80°C @ 101.3 kPa	1	ECHA
Boiling point	>300°C	1	ECHA
Density	967 kg/m^3@ 20°C	1	ECHA
Vapour pressure	0 Pa @ 25°C	1	ECHA
Partition coefficient (log K_{ow})	>6 (experimental)	1	ECHA
Water solubility	0.00012 g/L @ 20°C	2	ECHA
Viscosity	805.87 mPa.s @ 20°C	1	ECHA

4. DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for amides, tall oils fatty, N,N-bis(hydroxyethyl).

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No

Convention, Protocol or other international control	Listed Yes or No?
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5. ENVIRONMENTAL FATE SUMMARY

A. Summary

Oleamide DEA is readily biodegradable, has a moderate potential to sorb to sediments and soil, and a low potential to bioaccumulate.

B. Biodegradation

Oleamide DEA is readily biodegradable. In an OECD 301 D test, degradation was 70% after 28 days (ECHA) [Kl. score = 1]. In an OECD 301 B test, degradation was 79% after 14 days and 86% after 28 days (ECHA) [Kl. score = 1]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

C. Environmental Distribution

No experimental data are available for Oleamide DEA. Using KOCWIN v2.00, the estimated K_{oc} values for the individual components were calculated using the molecular connectivity index (MCI) approach. The final K_{oc} value was calculated on a weighted-average basis using the mole fractions of the individual components. The final K_{oc} value is 1,717 L/kg.

When released to the environment, oleamide DEA, based on its low water solubility and high K_{oc} value, is likely to adsorb to soil or sediment and has a low potential for mobility.

D. Bioaccumulation

There are no bioaccumulation studies on oleamide DEA. The bioaccumulation potential of oleamide DEA was estimated using BCFBAF v3.01. The final BCF was calculated on a weighted-average basis using the mole fractions of all individual components. The calculated BCF was 112.53 L/kg, indicating a low potential for bioaccumulation (ECHA).

6. HUMAN HEALTH HAZARD ASSESSMENT

Human health toxicity data were obtained from ECHA, unless another source is explicitly cited.

A. Summary

The acute toxicity of oleamide DEA is low by the oral and dermal routes. It is a skin and eye irritant. However, it is not considered a skin sensitiser. It is not toxic via repeated doses; has no reported reproductive or developmental effects; and, is not considered genotoxic or carcinogenic.

B. Acute Toxicity

Oleamide DEA is not considered acutely toxic via oral route of exposure, with an LD_{50} of 10,000 mg/kg in male Sprague-Dawley rats [Kl. Score = 2].

There are no acute inhalation toxicity studies on oleamide DEA. Based on the physical properties of the substance (i.e., vapour pressure), the studies did not need to be conducted (ECHA).

A study was conducted to determine the acute dermal toxicity of oleamide DEA and a read-across substance [amides, C8-18 (even-numbered)] in male and female albino rabbit. No adverse effect was observed. The acute dermal LD_{50} was found to be > 2,000 mg/kg bw [Kl. Score = 2].

C. Irritation

Based on the available data, the test substance is considered irritating to both the skin and eyes. The available in vivo studies demonstrate:

- Clear irritation response following semi-occlusive exposure to the test substance for 24 hours. The data support a classification as Skin Irrit. 2 - H315 (causes skin irritation) according to CLP (EC 1272/2008) criteria [Kl. Score =1].
- Undiluted test substance showed irritation to rabbit eyes and supports classification as Eye Irrit. 2 – H319 (causes serious eye irritation) according to CLP (EC 1272/2008) criteria [Kl. Score = 1].

D. Sensitisation

The test substance is not expected to be a skin sensitiser based on a negative in vivo skin sensitisation study conducted on a structurally similar substance [Kl. Score = 1]. Therefore, no classification is required for sensitisation according to CLP (EC 1272/2008) criteria. There are no data on the respiratory sensitization potential of the substance.

E. Repeated Dose Toxicity

Oral

An oral subacute study was conducted to determine the repeated dose oral toxicity of oleamide DEA and the read across substance [amides, C12-18 (even-numbered)] to rats. Groups of 10 male and 10 female rats were orally gavaged with the substance diluted in olive oil, 5 d/wk for 28 d at doses of 0, 70, 250, 750 (Days 1-14) and 1500 (Days 15-28) mg/kg bw/d. Clinical signs, bodyweight, hematology, clinical chemistry, urinalysis, gross and microscopic pathology were recorded. Additional groups of 5 male and 5 female rats were kept for a 4-month recovery period. No treatment-related adverse effects were observed at any of the doses. Changes in the forestomach at some doses including controls were attributed to the use of olive oil and found to be reversible after end of exposure. Under the conditions of the study, the 28-day NOAEL to rats was therefore considered to be greater than 750 mg/kg bw/day (Potokar, 1983 as cited in ECHA) [Kl. Score = 2].

Based on the findings of the oral subacute study, the test substance is not considered to meet the requirements for repeated dose toxicity classification according to CLP (EC 1272/2008) criteria.

Inhalation

There are no data to evaluate the repeated dose toxicity classification for the inhalation exposure route.

Dermal

A 2-year study was conducted to evaluate the effects of chronic exposure to the test substance in F344/N rats. Groups of 50 male and 50 female rats were dermally exposed to 0, 50 or 100 mg/kg bw/day in ethanol at a frequency of 5 d/wk for a period of 104 weeks. Survival, clinical findings, body weight and histopathology of different organs were assessed at specific time intervals. Survival of the dosed male and female rats was similar to that of the vehicle control groups. The mean body weights of males and females (Week 24 onwards) were reduced than those of the vehicle control group at 100 mg/kg bw/day. A dose dependent increase in irritation (mild to moderate) and non-neoplastic lesions (minimal to moderate) of the skin were observed at the site of application in all animals. The non-neoplastic lesions included epidermal hyperplasia, sebaceous gland hyperplasia, hyperkeratosis, parakeratosis, chronic active dermal inflammation and ulcer. No significant neoplastic lesions or evidence of carcinogenic activity was observed at any tested dose levels in skin, testis and thyroid gland. Under the conditions of the study, the NOAEL for systemic effects can be considered to be 50 mg/kg bw/d and the LOAEL for local effects can be considered at the lowest dose of 50 mg/kg bw/d (Irwin, 1999 as cited in ECHA) [Kl. Score = 1].

Based on the findings of a chronic dermal study in rat (NOAEL of 50 mg/kg bw/day for systemic effects and LOAEL of 50 mg/kg bw/day for local effects), the test substance is not considered to meet the requirements for repeated dose toxicity classification according to CLP (EC 1272/2008) criteria.

F. Genotoxicity

The test substance (oleamide DEA) and read across substance (amides, C8-18 (even numbered)) were negative in short-term in vitro and in vivo genotoxicity tests. Therefore, no classification is required for this endpoint according to CLP (EC 1272/2008) criteria.

In Vitro Studies

The *in vitro* studies conducted for this substance are described in Table 3. The referenced studies indicate that the substance is not mutagenic or genotoxic *in vitro*.

Table 3 In vitro Genotoxicity Studies

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
In vitro gene mutation study in bacteria (*S. typhimurium* TA97, TA98, TA100 and TA1535)	-	-	2	Irwin, 1999**
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	Irwin, 1999**
Bacterial reverse mutation (S. typhimurium and E. coli strains)	-	-	1	Verspeek-Rip, 2014**

*+, positive; -, negative.
** As cited in ECHA.

In Vivo Studies

A study was conducted to evaluate the potential of the test material to induce micronuclei in B6C3F1 mice. Under the conditions of the study, the test substance did not increase the frequencies of micronucleated normochromatic erythrocytes (NCEs) in peripheral blood of both male and female mice at the end of 13 weeks [Kl. Score = 1].

G. Carcinogenicity

Oral

No studies are available.

Inhalation

No studies are available.

Dermal

Rodent tests indicate that the substance is not carcinogenic by the dermal route. A study was conducted to evaluate the effects of chronic exposure to the test substance in B6C3F1 mice. Under the test conditions, no evidence of carcinogenic activity was observed with the test substance at any tested dose levels in mice [Kl. Score = 1]. A study was conducted to evaluate the effects of chronic exposure to the test substance in F344/N rats. Under the test conditions, no evidence of carcinogenic activity was observed with the test substance at any tested dose levels in rats [Kl. Score = 1].

H. Reproductive Toxicity

No studies were available to assess the effects of the substance on reproduction.

I. Developmental Toxicity

No adverse developmental effects were observed following administration of 1,000 mg/kg bw day to pregnant Sprague-Dawley rats (Kl. Score = 2).

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

The lowest NOAEL from these studies is a 750 mg/kg bw/day based on bodyweight, hematology, clinical chemistry, urinalysis, gross and microscopic pathology in male and female rats from a 28-day oral gavage study (Potokar, 1983 as cited in ECHA). The NOAEL of 750 mg/kg-day will be used for determining the oral reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 750/(10 x 10 x 1 x 10 x 1) = 750/1000 = 0.75 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.75 x 70 x 0.1)/2 = 2.63 mg/L

Cancer

Oleamide DEA was not carcinogenic to rats or mice in chronic oral studies. Therefore, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Oleamide DEA does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Oleamide DEA has moderate toxicity to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on oleamide DEA.

Table 4 Acute Aquatic Toxicity Studies on Oleamide DEA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Danio rerio	96-hour LC_{50}	5.1	1	ECHA
Daphnia magna	48-hour EC_{50}	3.2	2	ECHA
Desmodesmus subspicatus	72-hour EC_{50}	18.6	2	ECHA

Chronic Studies

The 28-day NOEC to *Oncorhynchus mykiss* in a fish chronic toxicity study is 0.32 mg/L [nominal] and 0.26 mg/L [measured] (ECHA) [Kl. score = 2].

The 21-day NOEC in a *Daphnia* reproduction test is 0.1 mg/L [nominal] and 0.07 mg/L [measured] (ECHA) [Kl. score = 2].

The 72-hour EC_{10} to *Desmodesmus subspicatus* is 1.4 mg/L (ECHA) [Kl. score = 2].

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

The PNEC calculations for oleamide DEA follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (5.1 mg/L), invertebrates (3.2 mg/L), and algae (18.6 mg/L). Results from chronic studies are available for fish (0.26 mg/L), invertebrates (0.07 mg/L), and algae (1.4 mg/L). On the basis that the data consists of short-term and long-term results for three trophic levels, an assessment factor of 10 has been applied to the lowest reported NOEC or EC_{10} value of 0.07 mg/L for invertebrates. The $PNEC_{water}$ is 0.007 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.18 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (33.78/1280) \times 1000 \times 0.007$
$= 0.18$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 68.68/1000 \times 2400]$
$= 33.78\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 1{,}717 \times 0.04$
$= 68.68$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for the substance calculated from EPISuite™ using the MCI approach is 1,717 L/kg .
f_{oc} = fraction of organic carbon in sediment = 0.04 [default]

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.16 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (34.34/1500) \times 1000 \times 0.007$
$= 0.16$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3) = 34.34 m^3/m^3 [calculated]
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]

And:
$Kp_{soil} = K_{oc} \times f_{oc}$
$= 1717 \times 0.02$
$= 34.34$ m^3/m^3

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for oleamide DEA based on the molecular connectivity index (MCI) is 1,717 L/kg (ECHA).
F_{oc} = fraction of organic carbon in soil = 0.02 [default].

8. CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Oleamide DEA is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on an estimated BCF value of 113 L/kg, oleamide DEA does not meet the criteria for bioaccumulation.

The lowest chronic NOEC or EC_{10} value for oleamide DEA is <0.1 mg/L. Thus, oleamide DEA meets the criteria for toxicity.

The overall conclusion is that oleamide DEA is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for oleamide DEA.

9. SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Amides, tall oils fatty, N,N-bis(hydroxyethyl)	68155-20-4	Not a PBT	No	No	No	No	No	Yes	2	2	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 2 – Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk..

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10. REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
BCFBAF	bioconcentration factor/bioaccumulation factor
CLP	Classification, Labelling and Packaging
COC	constituent of concern

DEA	diethanolamine
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
kg/m^3	kilograms per cubic metre
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/kg bw/day	mg of substance per kg of body weight administered per day.
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mPa.s	millipascal second
NCE	normochromatic erythrocyte
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases

UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
USEPA	United States Environmental Protection Agency

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
					0	30	0	30	0	30	
Amides, tall-oil fatty, N,N-bis(hydroxyethyl)	68155-20-4	5.10E+00	1.50E+01	6.80E-01	6.80E-02	1.70E-02	6.80E-04	1.70E-04	1.36E-05	3.40E-06	7.00E-03

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

Santos

Tier 3 Assessments

Qualitative and Quantitative Tier 3 Assessment

Dialuminium Chloride Pentahydroxide

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Dialuminium chloride pentahydroxide (also known as aluminium chlorohydrate) is a component in a Water Management Facility (WMF) product used as a coagulant during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals – Tier 3 Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Aluminium chlorohydrate Water	12042-91-0 7732-18-5	Coagulant	20000 L

CAS No = Chemical Abstracts Service Number
L = litre

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Since an Australian Drinking Water Guideline (ADWG) Value is available (see **Table 2**), toxicological reference values (TRVs) were not derived for the chemical. A detailed discussion of the drinking water guideline values is presented in **Attachment 2**.

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Aluminium chlorohydrate (12042-91-0)	Aluminium; chloride	0.2 mg/L (aesthetics); 250 mg/L (aesthetics)

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of TRVs was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Aluminium chlorohydrate (12042-91-0)	-	-	-	0.0008[a]

[a] PNECwater for aluminium chlorohydrate is the Australian and New Zealand Guidelines (ANZG) Water Quality Guideline – Freshwater Trigger Value for aluminium
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Polyaluminium coagulants, which have been developed for water treatment applications, have the general formula $(Al_n(OH)_mCl(3_{n-m})_x)$. The length of the polymerised chain, molecular weight, and the number of ionic charges is determined by the degree of polymerisation (Gebbie, 2001). The molecular structure of dialuminium chloride pentahydroxide (n=2; m=5) is presented in **Figure 1.**

Figure 1 Molecular Structure of Dialuminium Chloride Pentahyroxide[2]

Dialuminium chloride pentahydroxide is very soluble in water and will dissociate to form aluminium hydroxide species and chloride ions. Biodegradation is not applicable to dialuminium chloride pentahydroxide. Both chloride ions and aluminium hydroxide ionic species can be found naturally in the environment. The aluminium hydroxide hydrolysis products will adsorb to colloidal matter.

Fish accumulate aluminium in and on the gill, and it has been suggested that the rate of transfer of aluminium into the body is either slow or negligible under natural environmental conditions (Spry and Wiener, 1991). Chloride ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Thus, dialuminium chloride pentahydroxide is not expected to bioaccumulate in aquatic organisms.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for dialuminium chloride pentahydroxide is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that dialuminium chloride pentahydroxide is not a PBT substance.

[2] Source https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID0051609

Human Health Hazards

Dialuminium chloride pentahydroxide has low acute toxicity by the oral and dermal routes. It is non-irritating to the skin and slightly irritating to the eyes. It is not a skin sensitiser.

No systemic, reproductive or developmental toxi/city was seen in rats at oral doses up to 1,000 milligrams per kilogram day (mg/kg-day) aluminium hydroxychloride (a structurally similar compound) in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Dialuminium chloride pentahydroxide is not genotoxic.

Toxicological reference values were not derived for dialuminium chloride pentahydroxide. The ADWG values for aluminium (acid-soluble) is 0.2 milligrams per litre (mg/L) based on aesthetics. ADWG has concluded that there is insufficient data to set a guidance value based on health considerations (ADWG, 2011). The ADWG value for chloride is 250 mg/L based on aesthetics (ADWG, 2011).

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the treatment process described in **Attachment 1**, dialuminium chloride pentahydroxide is removed with Actiflo sludge (solid waste) during water treatment. As a result, this chemical is not directed to the permeate or brine waste streams and would not be present in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

In the aquatic environment, aluminium compound toxicity is intimately related to ambient pH; changes in ambient acidity may affect aluminium compound solubility, dissolved aluminium compound speciation and organism sensitivity to aluminium compounds. In acute toxicity tests, the pH significantly alters the speciation and therefore bioavailability of the aluminium such that acutely toxic concentrations occur below a pH of 6 but that above 6 the bioavailable concentration necessary to achieve immobilisation in an acute study cannot be achieved.

Toxicity testing on a similar aluminium salt compound (sulfuric acid, aluminium salt (3:2), octadecahydrate [CAS No. 7784-31-8]) identified a low toxicity concern for terrestrial invertebrates.

In developing a water quality guideline for aluminium (ANZG, 2018), the screened freshwater toxicity data were separated into those conducted at pH >6.5 and those at pH <6.5. The guideline for freshwater with a pH > 6.5 is 55 micrograms per litre (µg/L). This is identified as a moderate reliability trigger level. A freshwater low-reliability trigger value of 0.8 µg/L was derived for a pH < 6.5. This low-reliability value should only be used as an indicative interim working level.

No experimental toxicity data on sediment or soil organisms are available. Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics, such as dialuminium chloride pentahydroxide. Thus, the equilibrium partitioning method cannot be used to calculate PNECs for soil or sediment. Based on its properties, dialuminium chloride pentahydroxide is not expected to significantly adsorb to soil or sediment, and the assessment of these compartments is covered by the aquatic assessment.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to dialuminium chloride pentahydroxide that may occur during water treatment activities. The risk characterisation evaluates the toxicity of dialuminium chloride pentahydroxide and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, dialuminium chloride pentahydroxide is not directed to the permeate or brine waste streams and would not be present in permeate, brine or treated water. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), dialuminium chloride pentahydroxide does not meet the criteria for persistence or bioaccumulation. Further, this chemical is not directed to the permeate or brine waste streams and would not be present in permeate, brine or treated water. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 4** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 4 Evaluation of Uncertainty – Dialuminium Chloride Pentahydroxide

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in the water treatment process were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Hazard Assessment –COPC concentrations	Concentrations of COPCs evaluated in the quantitative risk assessment were assumed to be 100 percent of mass used in the water treatment process. This is a conservative assumption for chemicals that may degrade rapidly or volatilise.	Medium	This assumption may overestimate the calculated risks to receptors.
Toxicity Assessment	The absence of terrestrial toxicity data and the lack of a Koc value to calculate a PNEC in soil or sediment.	Medium	Medium to high potential to underestimate risks.

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Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Aluminium Chlorohydrate 50%	Aluminium chlorohydrate Water	12042-91-0 7732-18-5	48-50% 50-52%	Aluminium Chlorohydrate	REDOX	Reverse Osmosis	10000L	50%	20000L	50%	13-17L/hour	50%	150000L	coagulant

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
L = litres
L/hour = litre per hour
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millillitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration
				(mg/L)	Permeate notes	(mg/kg)	(mg/kg)	(mg/L)
Aluminium Chlorohydrate 50%	Aluminium chlorohydrate	12042-91-0	Removed with Actiflo sludge (solid waste)	NA	This product is not directed to the permeate stream.	NA	NA	NA
	Water	7732-18-5		NA	This product is not directed to the permeate stream.	NA	NA	NA

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
L = litres
L/hour = litre per hour
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millillitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Notes
Aluminium Chlorohydrate 50%	Aluminium chlorohydrate	12042-91-0	This product not directed to brine dams.
	Water	7732-18-5	This product not directed to brine dams.

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
L = litres
L/hour = litre per hour
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millillitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

DIALUMINIUM CHLORIDE PENTAHYDROXIDE

This dossier on dialuminium chloride pentahydroxide presents the most critical studies pertinent to the risk assessment of dialuminium chloride pentahydroxide in water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Dialuminium chloride pentahydroxide was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Dialuminium chloride pentahydroxide was assessed as a tier 3 chemical for acute toxicity and as a tier 1 chemical for chronic toxicity. Therefore, dialuminium chloride pentahydroxide is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Dialuminium chloride pentahydroxide is very soluble in water and will dissociate to form aluminium hydroxide species and chloride ions. Biodegradation is not applicable to dialuminium chloride pentahydroxide. The aluminium hydroxide hydrolysis products will adsorb to colloidal matter. Dialuminium chloride pentahydroxide is not expected to bioaccumulate in aquatic organisms. Dialuminium chloride pentahydroxide has low acute toxicity by the oral and dermal routes. It is non-irritating to the skin and slightly irritating to the eyes. It is not a skin sensitiser. No systemic, reproductive or developmental toxicity was seen in rats at oral doses up to 1,000 mg/kg-day aluminium hydroxychloride (a structurally similar compound) in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Dialuminium chloride pentahydroxide is not genotoxic. The Australian drinking water guideline (ADWG) values for aluminium (acid-soluble) is 0.2 mg/L based on aesthetics. ADWG has concluded that there is insufficient data to set a guidance value based on health considerations. The ANZECC water quality guideline (ANZECC & ARMCANZ, 2000) used acute and chronic laboratory toxicity data for the derivation of trigger values for aluminium, which are 55 µg/L at pH >6.5 and 0.8 µg/L at pH of <6.5.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Dialuminium chloride pentahydroxide

CAS RN: 12042-91-0

Molecular formula: $Al_2ClH_5O_5$; general formula $Al(OH)_x(Cl)_{(3-x)}$ with x between 2.3 and 2.6

Molecular weight: 174.45

Synonyms: Dialuminium chloride pentahydroxide; dialuminium chloride pentahydroxide; aluminium chlorohydroxide; aluminium hydroxychloride dehydrate; aluminium chloride hydroxide, dihydrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Dialuminium Chloride Pentahydroxide

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid; fine flakes	1	ECHA
Melting Point	No melting point below 400°C could be determined.	1	ECHA
Boiling Point	No boiling point below 400°C could be determined.	1	ECHA
Density	1.95 g/cm^3 @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	-	-	-
Water Solubility	>1,000 g/L @ 20°C (sample pH was 3.3)	1	ECHA
Auto flammability	Not auto flammable.	1	ECHA

Polyaluminium coagulants, which have been developed for water treatment applications, have the general formula $(Al_n(OH)_mCl_{(3n-m)})_x$. The length of the polymerised chain, molecular weight, and the number of ionic charges is determined by the degree of polymerisation. The polyaluminium coagulants include polyaluminium chloride (n=2; m=3), dialuminium chloride pentahydroxide (n=2; m=5), and polydialuminium chloride pentahydroxide (similar to dialuminium chloride pentahydroxide) (Gebbie, 2001).

On hydrolysis, various mono- and polymeric species are formed, with an important cation being $Al_{13}O_4(OH)_{24}^{7+}$. A less predominant species is $Al_8(OH)_{20}^{4+}$.

Depending on the pH, the following reaction takes place (Gebbie, 2005):

$$Al_2(OH)_5Cl \rightarrow Al_2(OH)_5^+ + Cl^- + H_2O \rightarrow 2Al(OH)_3 + H^+ + Cl^-$$

This reaction will typically take place at a water pH of 5.8 to 7.5. Within this pH, colour and the colloidal matter are removed by adsorption onto/within the metal hydroxide hydrolysis products that are formed (Gebbie, 2005).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for dialuminium chloride pentahydroxide.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Dialuminium chloride pentahydroxide is very soluble in water and will dissociate to form aluminium hydroxide species and chloride ions. Biodegradation is not applicable to dialuminium chloride pentahydroxide. The aluminium hydroxide hydrolysis products will adsorb to colloidal matter. Dialuminium chloride pentahydroxide is not expected to bioaccumulate in aquatic organisms.

B. Biodegradation

Biodegradation is not applicable to dialuminium chloride pentahydroxide.

C. Bioaccumulation

Fish accumulate aluminium in and on the gill, and it has been suggested that the rate of transfer of aluminium into the body is either slow or negligible under natural environmental conditions (Spry and Wiener, 1991). The initial uptake of aluminium by fish occurs mainly on the gill mucous layer (Wilkinson and Campbell, 1993); both mucus and bound aluminium may be rapidly eliminated following exposure. Roy (1999) calculated the BCFs in fish to range from 400 to 1,365.

The BCF for *Daphnia magna* varied from 10,000 at pH 6.5 to 0 at pH 4.5, based on the results of Havas (1985). Most of the metal appears to be adsorbed to external surfaces and is not internalised (Havas, 1985; Frick and Hermann, 1990).

The accumulation of aluminium by the algae *Chlorella pyrenoidosa* increased with the concentration of inorganic monomeric aluminium (Parent and Campbell, 1994). A comparison of assays performed at different pH values but the same concentration of aluminium showed suppression of that aluminium accumulation at low pH.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Dialuminium chloride pentahydroxide has low acute toxicity by the oral and dermal routes. It is non-irritating to the skin and slightly irritating to the eyes. It is not a skin sensitiser. No systemic, reproductive or developmental toxicity was seen in rats at oral doses up to 1,000 mg/kg-day aluminium hydroxychloride (a structurally similar compound) in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Dialuminium chloride pentahydroxide is not genotoxic.

B. Acute Toxicity

No oral acute toxicity studies are available for dialuminium chloride pentahydroxide. The oral LD_{50} of aluminium hydroxychloride in rats is >2,000 mg/kg (ECHA) [Kl. score = 2].

The dermal LD_{50} of dialuminium chloride pentahydroxide in rats is >2,000 mg/kg (ECHA) [Kl. score = 2].

C. Irritation

No skin irritation studies are available for dialuminium chloride pentahydroxide. Application of 0.5 mL of aluminium hydroxychloride to the skin of rabbits for 4 hours under semi-occlusive conditions was not irritating. The mean of the 24, 48 and 72 hour scores were zero for both erythema and edema (ECHA). [Kl. score = 1]

Dialuminium chloride pentahydroxide was slightly irritating to the eyes of rabbits. The mean of the 24, 48 and 72-hour conjunctival redness scores was 1.00; all other parameters were zero (ECHA). [Kl. score = 1]

D. Sensitisation

Dialuminium chloride pentahydroxide was not a skin sensitiser in a guinea pig maximisation test (ECHA) [Kl. score = 1].

E. Repeated Dose Toxicity

<u>Oral</u>

No studies are available on dialuminium chloride pentahydroxide.

Aluminium chloride, basic (aluminium hydroxychloride) was tested in a combined repeated dose toxicity and reproductive/developmental screening toxicity (OECD 422) study. Male and female Wistar rats were dosed by oral gavage with 0, 40, 200 or 1,000 mg/kg aluminium chloride, basic; these doses correspond to 0, 3.6, 18 or 90 mg/kg-day aluminium. There were no effects in the females at any dose level. In males, there were effects indicative of stomach irritation at the high-dose; no other effects were noted. The NOAEL for systemic effects in this study is 1,000 mg/kg-day, the highest dose tested. The NOAEL for localised effects (site-of-contact) is 200 mg/kg-day (ECHA). [Kl. score = 2]

Inhalation

No adequate studies were located.

Dermal

No studies are available.

F. Genotoxicity

In Vitro Studies

Dialuminium chloride pentahydroxide was not mutagenic to *S. typhimurium* strains TA98, TA100, TA1535, TA1537 and *E. coli* strain WP2*uvr*A in the absence or presence of metabolic activation (ECHA). [Kl. score = 1]

The *in vitro* genotoxicity studies on the structurally similar compound aluminium hydroxychloride is shown in Table 3.

Table 3 *In Vitro* Genotoxicity Studies on Aluminium Hydroxychloride

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (S. typhimurium and E. coli strains)	-	-	1	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	ECHA
Micronucleus (peripheral human lymphocytes)	-	-	1	ECHA

*+, positive; -, negative

In Vivo Studies

Male and female NMRI mice were given an oral gavage dose of 0 or 2,000 mg/kg dialuminium chloride pentahydroxide on two consecutive days. There were no increases in the frequency of micronucleated polychromatic erythrocytes in the bone marrow of the treated mice compared to the controls (ECHA). [Kl. score = 1]

G. Carcinogenicity

No studies are available.

H. Reproductive/Developmental Toxicity

No studies are available for dialuminium chloride pentahydroxide.

Aluminium chloride, basic (aluminium hydroxychloride) was tested in a combined repeated dose toxicity and reproductive/developmental screening toxicity (OECD 422) study. Male and female Wistar rats were dosed by oral gavage with 0, 40, 200 or 1,000 mg/kg aluminium chloride, basic; these doses correspond to 0, 3.6, 18 or 90 mg/kg-day aluminium. There was no reproductive or

developmental toxicity at any dose level. The NOAELs for reproductive and developmental toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA). [Kl. score = 1]

I. Derivation of Toxicological Reference and Drinking Water Guidance Values

Toxicological reference values were not derived for dialuminium chloride pentahydroxide.

The ADWG value for aluminium (acid-soluble) is 0.2 mg/L based on aesthetics. ADWG has concluded that there is insufficient data to set a guidance value based on health considerations (ADWG, 2011).

The ADWG value for chloride is 250 mg/L based on aesthetics (ADWG, 2011).

J. Human Health Hazard Assessment of Physico-Chemical Properties

Dialuminium chloride pentahydroxide does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

In the aquatic environment, aluminium compound toxicity is intimately related to ambient pH; changes in ambient acidity may affect aluminium compound solubility, dissolved aluminium compound speciation and organism sensitivity to aluminium compounds. Toxicity testing on a similar aluminium salt compound identified a low toxicity concern for terrestrial invertebrates.

B. Aquatic Toxicity

Acute Studies on Aluminium Polychlorohydrate

Table 4 lists the results of acute aquatic toxicity studies conducted on aluminium salts.

Table 4 Acute Aquatic Toxicity Studies on Aluminium Salts

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Zebrafish *(Danio rerio)*	96-hour LC_{10}	142 nominal (as dissolved aluminum 0.58)	2	ECHA
Zebrafish	96-hour LC_{50}	186 nominal (as dissolved aluminum 1.39)	2	ECHA
Zebrafish	96-hour EC_{50}	>0.357* as Dis Al	1	ECHA
Water Flea *(Daphnia magna)*	48-hour EC_{50}	98 nominal (as dissolved aluminum <0.1)**	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Water Flea	48-hour EC_{50}	38*** nominal (as dissolved aluminum 1.26)	2	ECHA
Pseudokidrchneriella subcapitata	72-hour EC_{50} growth rate	14 nominal (as dissolved aluminum 0.24)	1	ECHA

*NOEC was >1,000 mg/L. pH of the test media was maintained at 7.5.
**Toxicity is driven by other causes than dissolved aluminium.
*** Value for dialuminium chloride pentahydroxide.

The pH significantly alters the speciation and therefore bioavailability of the aluminium such that acutely toxic concentrations occur below a pH of 6 but that above 6 the bioavailable concentration necessary to achieve immobilisation in an acute study cannot be achieved (ECHA).

Data used by ANZECC for Aluminium water quality guideline

In developing a water quality guideline for aluminium (ANZECC & ARMCANZ, 2000), ANZECC separated the screened freshwater toxicity data into those conducted at pH >6.5 and those at pH <6.5. These data are summarised below (it should be noted that only the acute toxicity data was used to derive a water quality guideline).

Freshwater pH >6.5:

Fish

The 48-96 hour LC_{50} values for 5 species were 600 to 106,000 µg/L (the lowest value was for *Salmo salar*). The chronic 8- to 28-day NOEC equivalents[1] from seven species were 34-7,100 µg/L. The lowest measured chronic value was an 8-day LC_{50} for *Micropterus* species of 170 µg/L.

Amphibian

The 96-hour LC_{50} values for *Bufo americanus* were 860-1,660 µg/L. The chronic 8-day LC_{50} for *Bufo americanus* was 2,280 µg/L.

Crustacean

The 48-hour LC_{50} values for one species were 2,300-36,900 µg/L. The chronic 7- to 28-day NOECs were 136-1,720 µg/L.

Algae

The 96-hour EC_{50} values were 460-570 µg/L based on population growth. The NOECs for two species were 800-2,000 µg/L.

Freshwater pH<6.5 (all between pH 4.5 and 6.0):

Fish

The 24-96-hour LC_{50} values for two species were 15-4,200 µg/L (the lowest value was for *Salmo trutta*). The 21- to 42-day LC_{50} values were 15-105 µg/L.

Amphibian

The 96- to 120-day LC_{50} values were 540-2,670 µg/L; the absolute range was 400-5,200 µg/L.

Algae

The NOEC from one species was 2,000 µg/L based on growth.

[1]Chronic toxicity values were a mixture of LC/EC_{50} LOEC, MATC, and NOEC values; where stated, these were converted to NOEC equivalents.

C. Terrestrial Toxicity

A study equivalent to the earthworm acute toxicity (OECD TG 207) test was conducted on sulfuric acid, aluminium salt (3:2), octadecahydrate (CAS No. 7784-31-8). The 14-day LC_{50} to earthworm *Eisenia andre*i was 316 mg/kg soil dry weight (van Gestel and Hoogerwerf, 2001; ECHA). [Kl. score = 2]

D. Calculation of PNEC

PNEC water

The ANZECC water quality guideline (ANZECC & ARMCANZ, 2000) used acute and chronic laboratory toxicity data for the derivation of trigger values for aluminium. The guideline for freshwater is: *"A freshwater moderate reliability trigger value of 55 µg/L for aluminium at pH >6.5 using the statistical distribution method (Burr distribution as modified by SCIRO, Section 8.3.3.3) with 95% protection and an ACR of 8.2."*

"A freshwater low-reliability trigger value of 0.8 µg/L was derived for aluminium at pH of <6.5 using an AF of 20 (essential element) on the low pH trout figure."

"The low-reliability figures should only be used as indicative interim working levels."

PNEC sediment

No experimental toxicity data on sediment organisms are available. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as dialuminium chloride pentahydroxide. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. Based on its properties, no adsorption of dialuminium chloride pentahydroxide to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No experimental toxicity data on soil organisms are available. The environmental distribution of dialuminium chloride pentahydroxide is dominated by its water solubility. Sorption of dialuminium chloride pentahydroxide should probably be regarded as a reversible situation, *i.e.*, the substance is not tightly nor permanently bound. K_{oc} and K_{ow} parameters do not readily apply to inorganics, such as dialuminium chloride pentahydroxide. Thus, the equilibrium partitioning methods cannot be used to calculate the $PNEC_{soil}$. Based on its properties, dialuminium chloride pentahydroxide is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Dialuminium chloride pentahydroxide is an inorganic compound that dissociates in water to form chloride ions and various species of aluminium hydroxide hydrolysis. Biodegradation is not applicable to dialuminium chloride pentahydroxide. Both chloride ions and aluminium hydroxide ionic species can be found naturally in the environment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic compound.

Fish accumulate aluminium in and on the gill, and it has been suggested that the rate of transfer of aluminium into the body is either slow or negligible under natural environmental conditions. Chloride ions are essential to all living organisms, and their intracellular, and extracellular concentrations are actively regulated. Thus, dialuminium chloride pentahydroxide and its dissociated ions are not expected to meet the criteria for bioaccumulation.

The lowest chronic NOEC value in fish for aluminium is <0.1 mg/L; thus, the dissolved aluminium from dialuminium chloride pentahydroxide meets the screening criteria for toxicity.

The overall conclusion is that dialuminium chloride pentahydroxide is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, dialuminium chloride pentahydroxide does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for dialuminium chloride pentahydroxide.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Dialuminium Chloride Pentahydroxide	12042-91-0	Not a PBT	No	No	NA	No	No	Yes	3	1	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AF	assessment factor
AICS	Australian Inventory of Chemical Substances
ANZECC	Australian and New Zealand Environment and Conservation Council
ARMCANZ	Agriculture and Resource Management Council of Australia and New Zealand
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
LD	lethal dose
LOEC	lowest observed effective concentration
MATC	maximum acceptable toxicant concentration
mg/kg	milligrams per kilogram

mg/L	milligrams per litre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NMRI	Naval Medical Research Institute
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
µg/L	micrograms per litre

Qualitative and Quantitative Tier 3 Assessment

Aluminium Hydroxychloride

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Aluminium hydroxychloride is a component in a Water Management Facility (WMF) product used as a coagulant during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals – Tier 3 Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Cationic Polymer[a] Aluminium Hydroxychloride Water	n/a 1327-41-9 7732-18-5	Polymer / coagulant	2 x 1000 L (IBC)

[a] Identity unknown. Read-across to polydiallyldimethylammonium chloride [polyDADMAC (CAS No. 26062-79-3)].
CAS No = Chemical Abstracts Service Number
IBC = intermediate bulk container
L = litre
n/a = not available

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Since an Australian Drinking Water Guideline (ADWG) Value is available (see **Table 2**), toxicological reference values (TRVs) were not derived for the chemical. A detailed discussion of the drinking water guideline values is presented in **Attachment 2**.

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Aluminium hydroxychloride (1327-41-9)	Aluminium; Chloride	0.2 mg/L (aesthetics); 250 mg/L (aesthetics)

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of TRVs was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Aluminium hydroxychloride (1327-41-9)	-	-	-	0.0008[a]

[a] $PNEC_{water}$ for aluminium hydroxychloride is the Australian and New Zealand Guidelines (ANZG) Water Quality Guideline – Freshwater Trigger Value for aluminium
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Polyaluminium coagulants, which have been developed for water treatment applications, have the general formula $(Al_n(OH)_mCl(3_{n-m})_x)$. The length of the polymerised chain, molecular weight, and the number of ionic charges is determined by the degree of polymerisation (Gebbie, 2001). The molecular structure of aluminium hydroxychloride is presented in **Figure 1**.

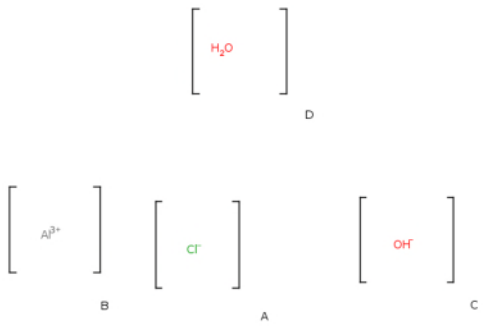

Figure 1 Molecular Structure of Aluminium Hydroxychloride[2]

Aluminium hydroxychloride is very soluble in water and will dissociate to form aluminium hydroxide species and chloride ions. Biodegradation is not applicable to aluminium hydroxychloride. Both chloride ions and aluminium hydroxide ionic species can be found naturally in the environment. The aluminium hydroxide hydrolysis products will adsorb to colloidal matter.

Fish accumulate aluminium in and on the gill, and it has been suggested that the rate of transfer of aluminium into the body is either slow or negligible under natural environmental conditions (Spry and Wiener, 1991). Chloride ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Thus, aluminium hydroxychloride is not expected to bioaccumulate in aquatic organisms.

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/1327-41-9

The Persistent, Bioaccumulative and Toxic (PBT) assessment for aluminium hydroxychloride is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that aluminium hydroxychloride is not a PBT substance.

Human Health Hazards

Aluminium hydroxychloride has low acute toxicity by the oral and dermal routes. It is non-irritating to the skin and slightly irritating to the eyes. It is not a skin sensitiser.

No systemic, reproductive or developmental toxicity was seen in rats at oral doses up to 1,000 milligrams per kilogram-day (mg/kg-day) aluminium hydroxychloride in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Aluminium hydrochloride is not genotoxic.

Toxicological reference values were not derived for aluminium hydroxychloride. The ADWG values for aluminium (acid-soluble) is 0.2 milligrams per litre (mg/L) based on aesthetics. ADWG has concluded that there is insufficient data to set a guidance value based on health considerations (ADWG, 2011). The ADWG value for chloride is 250 mg/L based on aesthetics (ADWG, 2011).

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the treatment process described in **Attachment 1**, aluminium hydroxychloride would be bound to the solids present in the oily water and removed during clarification. As a result, this chemical would not be present in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

In the aquatic environment, aluminium compound toxicity is intimately related to ambient pH; changes in ambient acidity may affect aluminium compound solubility, dissolved aluminium compound speciation and organism sensitivity to aluminium compounds. In acute toxicity tests, the pH significantly alters the speciation and therefore bioavailability of the aluminium such that acutely toxic concentrations occur below a pH of 6 but that above 6 the bioavailable concentration necessary to achieve immobilisation in an acute study cannot be achieved.

Toxicity testing on a similar aluminium salt compound (sulfuric acid, aluminium salt [3:2], octadecahydrate [CAS No. 7784-31-8]) identified a low toxicity concern for terrestrial invertebrates.

In developing a water quality guideline for aluminium (ANZG, 2018), the screened freshwater toxicity data were separated into those conducted at pH >6.5 and those at pH <6.5. The guideline for freshwater with a pH > 6.5 is 55 micrograms per litre (µg/L). This is identified as a moderate reliability trigger level. A freshwater low-reliability trigger value of 0.8 µg/L was derived for a pH < 6.5. This low-reliability value should only be used as an indicative interim working level.

No experimental toxicity data on sediment or soil organisms are available. Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics, such as aluminium hydroxychloride. Thus, the equilibrium partitioning method cannot be used to calculate PNECs for soil or sediment. Based on its properties, aluminium hydroxychloride is not expected to significantly adsorb to soil or sediment, and the assessment of these compartments is covered by the aquatic assessment.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to aluminium hydroxychloride that may occur during water treatment activities. The risk characterisation evaluates the toxicity of aluminium

hydroxychloride and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, aluminium hydroxychloride is not directed to the permeate or brine waste streams and would not be present in permeate, brine or treated water. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), aluminium hydroxychloride does not meet the criteria for persistence or bioaccumulation. Further, this chemical is not directed to the permeate or brine waste streams and would not be present in permeate, brine or treated water. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the

environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 4** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 4 Evaluation of Uncertainty – Aluminium Hydroxychloride

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in the water treatment process were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Hazard Assessment –COPC concentrations	Concentrations of COPCs evaluated in the quantitative risk assessment were assumed to be 100 percent of mass used in the water treatment process. This is a conservative assumption for chemicals that may degrade rapidly or volatilise.	Medium	This assumption may overestimate the calculated risks to receptors.
Toxicity Assessment	The absence of terrestrial toxicity data and the lack of a Koc value to calculate a PNEC in soil or sediment.	Medium	Medium to high potential to underestimate risks.

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Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
MAK MFC1 (multi floc coagulant)	Cationic Polymer	NA	20-40%	MAK MFC1	MAK Water Industrial	Oily Water Treatment Plant	1000L IBC		2 x 1000L (IBC)		0.8mg/L (AVG)			polymer / coagulant
	Aluminium Hydroxychloride	1327-41-9	40-60%											
	Water	7732-18-5	20-60%											

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
RO = reverse osmosis
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration
				(mg/L)	Permeate notes	(mg/kg)	(mg/kg)	(mg/L)
MAK MFC1 (multi floc coagulant)	Cationic Polymer	NA	Removed with oily water sludge (solid waste)	NA	Oily water is clarified to remove solids and oils then run through the RO system. The amount relative to flux of RO system is <1%. Therefore, the net on permeate quality is de minimis. Therefore, this chemical is not present in the permeate.	NA	NA	NA
	Aluminium Hydroxychloride	1327-41-9		NA	Oily water is clarified to remove solids and oils then run through the RO system. The amount relative to flux of RO system is <1%. Therefore, the net on permeate quality is de minimis. Therefore, this chemical is not present in the permeate.	NA	NA	NA
	Water	7732-18-5		NA		NA	NA	NA

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
RO = reverse osmosis
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Notes
MAK MFC1 (multi floc coagulant)	Cationic Polymer	NA	The oily water is clarified to seperate solids and oils; then run through the RO system. Estimate 5% residual in brine, the balance is sludge.
	Aluminium Hydroxychloride	1327-41-9	The oily water is clarified to seperate solids and oils; then run through the RO system. Estimate 5% residual in brine, the balance is sludge. Estimate that chemical will dissociate to aluminium (Al) and Cl- at 40% Al and 55% Cl-.
	Water	7732-18-5	

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
RO = reverse osmosis
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

ALUMINIUM HYDROXYCHLORIDE

This dossier on aluminium hydroxychloride presents the most critical studies pertinent to the risk assessment of aluminium hydroxychloride in water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Aluminium hydroxychloride was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. However, aluminium hydroxychloride was assessed as a tier 3 chemical for acute toxicity and as a tier 3 chemical for chronic toxicity. Therefore, aluminium hydroxychloride is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Aluminium hydroxychloride is very soluble in water and will dissociate to form aluminium hydroxide species and chloride ions. Biodegradation is not applicable to Aluminium hydroxychloride. The Aluminium hydroxide hydrolysis products will adsorb to colloidal matter. Aluminium hydroxychloride is not expected to bioaccumulate in aquatic organisms. Aluminium hydroxychloride has low acute toxicity by the oral and dermal routes. It is non-irritating to the skin and slightly irritating to the eyes. It is not a skin sensitiser. No systemic, reproductive, or developmental toxicity was seen in rats at oral doses up to 1,000 mg/kg-day Aluminium hydroxychloride in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Aluminium hydroxychloride is not genotoxic. The Australian drinking water guideline values for aluminium (acid-soluble) is 0.2 mg/L based on aesthetics. ADWG has concluded that there is insufficient data to set a guidance value based on health considerations. The ANZECC water quality guideline (2000) used acute and chronic laboratory toxicity data for the derivation of trigger values for Aluminium, which are 55 µg/L at pH >6.5 and 0.8 µg/L at pH of <6.5.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Aluminium(3+) ion dichloride hydroxide

CAS RN: 1327-41-9

Molecular formula: General formula $Al(OH)_x(Cl)_{(3-x)}$, with x ranging from >0 to 2.3 and typically being >0.5.

Molecular weight: variable

Synonyms: Aluminium hydroxychloride; polyaluminium chloride; aluminium chloride, basic; aluminium(3+) ion dichloride hydroxide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Aluminium Hydroxychloride (as Aqueous Solution)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear yellow liquid.	1	ECHA
Melting Point	<-90°C	1	ECHA
Boiling Point	70 – 170°C*	1	ECHA
Density	1.36 g/cm^3	1	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	>1,000 g/L @ 20°C (pH of sample was 2.4)	1	ECHA
Flash Point	No flash point was observed.	1	ECHA
Auto flammability	Not auto-ignitable	1	ECHA

*Assigned to boiling of water in the test sample.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for aluminium hydroxychloride.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Aluminium hydroxychloride is highly soluble and dissociates rapidly in aqueous solution. It is not expected to bioaccumulate and as an inorganic substance does not biodegrade. Further environmental fate details are provided below.

A. Summary

Aluminium hydroxychloride is very soluble in water and will dissociate to form aluminium hydroxide species and chloride ions. Biodegradation is not applicable to aluminium hydroxychloride. The aluminium hydroxide hydrolysis products will adsorb to colloidal matter. Aluminium hydroxychloride is not expected to bioaccumulate in aquatic organisms.

B. Biodegradation

Biodegradation testing is not relevant for this substance as it is inorganic in nature and expected to dissociate in the environment.

C. Bioaccumulation

Fish accumulate aluminium in and on the gill, and it has been suggested that the rate of transfer of aluminium into the body is either slow or negligible under natural environmental conditions (Spry and Wiener, 1991). The initial uptake of aluminium by fish occurs mainly on the gill mucous layer (Wilkinson and Campbell, 1993); both mucus and bound aluminium may be rapidly eliminated following exposure. Roy (1999) calculated the BCFs in fish to range from 400 to 1,365 L/kg.

The BCF for *Daphnia magna* varied from 10,000 L/kg at pH 6.5 to 0 at pH 4.5, based on the results of Havas (1985). Most of the metal appears to be adsorbed to external surfaces and is not internalised (Havas, 1985; Frick and Hermann, 1990).

The accumulation of aluminium by the algae *Chlorella pyrenoidosa* increased with the concentration of inorganic monomeric aluminium (Parent and Campbell, 1994). A comparison of assays performed at different pH values but the same concentration of aluminium showed suppression of that aluminium accumulation at low pH.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Aluminium hydroxychloride has low acute toxicity by the oral, dermal and inhalation routes. It is non-irritating to the skin, but severely irritating to the eyes. It is not a skin sensitiser. No systemic, reproductive or developmental toxicity was seen in rats at oral doses up to 1,000 mg/kg-day aluminium hydroxychloride in a combined repeated dose toxicity and reproductive/developmental toxicity screening (OECD 422) study. Aluminium hydroxychloride is not genotoxic.

B. Acute Toxicity

The oral LD_{50} of aluminium hydroxychloride in rats is >2,000 mg/kg (ECHA). [Kl. score = 2]

The 4-hour LC_{50} in rats is >5 mg/L as aerosol (ECHA). [Kl. score = 2]

The dermal LD_{50} of aluminium hydroxychloride in rats is >2,000 mg/kg (ECHA). [Kl. score = 2]

C. Irritation

Application of 0.5 mL of aluminium hydroxychloride to the skin of rabbits for 4 hours under semi-occlusive conditions was not irritating. The mean of the 24, 48 and 72 hour scores were zero for both erythema and edema (ECHA). [Kl. score = 1]

Instillation of 0.1 mL of aluminium hydroxychloride (low basicity) to the eyes of rabbits was severely irritating/corrosive. The mean of the 24, 48 and 72 hour scores were: 1.45 for corneal opacity; 0.89 for iridial lesions; 2.67 for conjunctival redness; and 2.55 for chemosis. The effects were not completely reversible within 21 days. One animal was killed due to the severity of the eye effects (ECHA). [Kl. score = 2]

D. Sensitisation

Aluminium hydrochloride was not a skin sensitiser in a guinea pig maximisation test using the Magnusson and Kligman method (ECHA). [Kl. score = 2]

E. Repeated Dose Toxicity

Oral

Aluminium hydroxychloride was tested in a combined repeated dose toxicity and reproductive/developmental screening toxicity (OECD 422) study. Male and female Wistar rats were dosed by oral gavage with 0, 40, 200, or 1,000 mg/kg aluminium hydroxychloride; these doses correspond to 0, 3.6, 18 or 90 mg/kg-day aluminium. There were no effects in the females at any dose level. In males, there were effects indicative of stomach irritation at the high-dose; no other effects were noted. The NOAEL for systemic effects in this study is 1,000 mg/kg-day, the highest dose tested. The NOAEL for localised effects (site-of-contact) is 200 mg/kg-day (ECHA). [Kl. score = 2]

Inhalation

No adequate studies are available.

Dermal

No studies are available.

F. Genotoxicity

The *in vitro* genotoxicity studies on aluminium hydroxychloride are presented in Table 3.

In Vitro Studies

Table 3 ***In Vitro*** **Genotoxicity Studies on Aluminium Hydroxychloride**

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* and *E. coli* strains)	-	-	1	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	-	1	ECHA
Micronucleus (peripheral human lymphocytes)	-	-	1	ECHA

*+, positive; -, negative

In Vivo Studies

No studies are available on aluminium hydroxychloride.

G. Carcinogenicity

No studies are available.

H. Reproductive/Developmental Toxicity

Aluminium hydroxychloride was tested in a combined repeated dose toxicity and reproductive/developmental screening toxicity (OECD 422) study. Male and female Wistar rats were dosed by oral gavage with 0, 40, 200 or 1,000 mg/kg aluminium hydroxychloride; these doses correspond to 0, 3.6, 18 or 90 mg/kg-day aluminium. There was no reproductive or developmental toxicity at any dose level. The NOAELs for reproductive and developmental toxicity is 1,000 mg/kg-day, the highest dose tested (ECHA). [Kl. score = 1]

I. Derivation of Toxicological Reference and Drinking Water Guidance Values

Toxicological reference values were not derived for aluminium hydroxychloride.

The Australian drinking water guideline values for aluminium (acid-soluble) is 0.2 mg/L based on aesthetics. ADWG has concluded that there is insufficient data to set a guidance value based on health considerations (ADWG, 2011).

The Australian drinking water guidance value for chloride is 250 mg/L based on aesthetics (ADWG, 2011).

J. Human Health Hazard Assessment Of Physico-Chemical Properties

Aluminium hydroxychloride does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Acute toxicity values for a variety of organisms are provided below and have, where possible, been converted to equivalence of aluminium. In general, acute toxicity values are pH dependent and range from LC50 of less than 1 mg/L to greater than 100 mg/L. Values used by ANZECC to derive water quality guidelines range from less than 1 to over 100 mg/L. Only acute values were used by ANZECC to derive the water quality trigger value of 55 µg/L for aluminium at pH >6.5.

B. Aquatic Toxicity

Acute Studies on Aluminium Polychlorohydrate

The 96-hr LC_{50} for aluminium polychlorohydrate in *Danio rerio* was determined to be 142 mg/L nominal. For dissolved aluminium, the 96-hr LC_{50} was 0.58 mg/L. A very steep concentration-effect relationship was observed for the test substance; this was due to the increase in solubility of aluminium as a result of the drop in pH from the increasing concentration of the test substance (ECHA). [Kl. score = 2]

The 96-hr LC_{50} for aluminium polychlorohydrate in *Danio rerio* was determined to be 186 mg/L nominal. For dissolved aluminium, the 96-hr LC_{50} was 1.39 mg/L, corresponding to 16.9 mg/L Total Al (measured values). A very steep concentration-effect relationship was observed for the test substance; this was due to the increase in solubility of aluminium as a result of the drop in pH from the increasing concentration of the test substance. Theoretically, 186 mg/L of aluminium polychlorohydrate reduced the pH of reconstituted water to a level which enabled 1.4 mg Al/L to be dissolved. (ECHA). [Kl. score = 2]

The 96-hr EC_{50} and NOEC for aluminium polychlorohydrate in *Danio rerio* were determined to be >0.357 mg/L measured as dissolved Al (equivalent to 91.5 Total Al). The NOEC was >1,000 mg/L nominal, which is equivalent to 91.5 mL Total Al. In this study, the pH of the test media was maintained at 7.5 (ECHA). [Kl. score = 1]

The 48-hr EC_{50} for aluminium polychlorohydrate in *Daphnia magna* is 98 mg/L nominal and 7.8 mg/L measured (ECHA) [Kl. score = 2]. Another study reported 48-hr EC_{50} values for aluminium chlorohydrate of 38 mg/L nominal and 3.45 mg/L measured (ECHA) [Kl. score = 2].

The 72-hr EC_{50} for growth rate in *Pseudokidrchneriella subcapitata* was 14 mg/L nominal, which was equivalent to 0.644 mg/L as Total Al. The average measured concentrations of dissolved Al were 0.24 mg/L at a pH between 7.1 and 8.4. The EC_{10} for growth rate was 0.14 mg/L as Total Al and 0.051 mg/L based on measured Al. The NOEC for growth inhibition was nominally 1.0 mg/L (0.046 mg/l based on Total Al) and <0.02 mg/L when based on measured Al (ECHA). [Kl. score = 1]

Data used by ANZECC for Aluminium water quality guideline

In developing a water quality guideline for aluminium (ANZECC & ARMCANZ, 2000), ANZECC separated the screened freshwater toxicity data into those conducted at pH >6.5 and those at pH <6.5. These data are summarised below (it should be noted that only the acute toxicity data was used to derive a water quality guideline).

Freshwater pH >6.5:

Fish

The 48-96 hour LC_{50} values for 5 species were 600 to 106,000 µg/L (the lowest value was for *Salmo salar*). The chronic 8- to 28-day NOEC equivalents[1] from seven species were 34-7,100 µg/L. The lowest measured chronic value was an 8-day LC_{50} for *Micropterus* species of 170 µg/L.

Amphibian

The 96-hour LC_{50} values for *Bufo americanus* were 860-1,660 µg/L. The chronic 8-day LC_{50} for *Bufo americanus* was 2,280 µg/L.

Crustacean

The 48-hour LC_{50} values for one species were 2,300-36,900 µg/L. The chronic 7- to 28-day NOECs were 136-1,720 µg/L.

Algae

The 96-hour EC_{50} values were 460-570 µg/L based on population growth. The NOECs for two species were 800-2,000 µg/L.

Freshwater pH<6.5 (all between pH 4.5 and 6.0):

Fish

The 24-96-hour LC_{50} values for two species were 15-4,200 µg/L (the lowest value was for *Salmo trutta*). The 21- to 42-day LC_{50} values were 15-105 µg/L.

Amphibian

The 96- to 120-day LC_{50} values were 540-2,670 µg/L; the absolute range was 400-5,200 µg/L.

Algae

The NOEC from one species was 2,000 µg/L based on growth.

[1]Chronic toxicity values were a mixture of LC/EC_{50} LOEC, MATC, and NOEC values; where stated, these were converted to NOEC equivalents.

C. Terrestrial Toxicity

A study equivalent to the earthworm acute toxicity (OECD TG 207) test was conducted on sulfuric acid, aluminium salt (3:2), octadecahydrate (CAS No. 7784-31-8). The 14-day LC_{50} to earthworm *Eisenia andre*i is 316 mg/kg soil dry weight (van Gestel and Hoogerwerf, 2001; ECHA). [Kl. score = 2]

D. Calculation of PNEC

The ANZECC and ARMCANZ water quality guideline (2000) used acute and chronic laboratory toxicity data for the derivation of trigger values for aluminium. The guideline for freshwater is: "A freshwater moderate reliability trigger value of 55 µg/L for aluminium at pH >6.5 using the statistical distribution method (Burr distribution as modified by SCIRO, Section 8.3.3.3) with 95% protection and an ACR of 8.2."

"A freshwater low-reliability trigger value of 0.8 µg/L was derived for aluminium at pH of <6.5 using an AF of 20 (essential element) on the low pH trout figure."

"The low-reliability figures should only be used as indicative interim working levels."

PNEC sediment

No experimental toxicity data on sediment organisms are available. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as aluminium hydroxychloride. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. Based on its properties, no adsorption of aluminium hydroxychloride to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No experimental toxicity data on soil organisms are available. The environmental distribution of aluminium hydroxychloride is dominated by its water solubility. Sorption of aluminium hydroxychloride should probably be regarded as a reversible situation, *i.e.*, the substance is not tightly nor permanently bound. K_{oc} and K_{ow} parameters do not readily apply to inorganics, such as aluminium hydroxychloride. Thus, the equilibrium partitioning methods cannot be used to calculate the $PNEC_{soil}$. Based on its properties, aluminium hydroxychloride is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Aluminium hydroxychloride is an inorganic compound that dissociates in water to form chloride ions and various species of aluminium hydroxide hydrolysis. Biodegradation is not applicable to aluminium hydroxychloride. Both chloride ions and aluminium hydroxide ionic species can be found naturally in the environment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic compound.

Fish accumulate aluminium in and on the gill, and it has been suggested that the rate of transfer of aluminium into the body is either slow or negligible under natural environmental conditions. Chloride ions are essential to all living organisms, and their intracellular, and extracellular concentrations are actively regulated. Thus, aluminium hydroxychloride and its dissociated ions are not expected to meet the criteria for bioaccumulation.

The lowest chronic NOEC value in fish for aluminium is <0.1 mg/L; thus, the dissolved aluminium from aluminium hydroxychloride meets the screening criteria for toxicity.

The overall conclusion is that aluminium hydroxychloride is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, aluminium hydroxychloride does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for aluminium hydroxychloride.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Aluminium Hydroxychloride	1327-41-9	Not a PBT	No	No	NA	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
ANZECC	Australian and New Zealand Environment and Conservation Council
ARMCANZ	Agriculture and Resource Management Council of Australia and New Zealand
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOEC	lowest observed effective concentration
MATC	maximum acceptable toxicant concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development

PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
µg/L	micrograms per litre

Qualitative and Quantitative Tier 3 Assessment

Cocoalkyl Dimethylbenzyl Ammonium Chloride

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Cocoalkyl dimethylbenzyl ammonium chloride (also known as alkyl dimethyl benzyl ammonium chloride [ADBAC]) is a component in a water treatment product used to provide corrosion resistance from microbial influenced corrosion in the steel flowlines and spinelines in the produced water management collection system. Process and usage information for this chemical is summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Percent Weight (%) in Product[1]
ADBAC	61789-71-7	Biocide	5

[1] Mid-point of range provided in SDS.
CAS No = Chemical Abstracts Service Number

The water treatment product could potentially be used for biocide treatment in FAPA but is currently not being used. Based on its use in other Santos project areas, dosage rates in water for this chemical in the biocide are in the range of 1×10^{-4} mg/L.

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. There are no carcinogenicity studies on ADBAC, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
ADBAC (61789-71-7)	2-yr rat oral	Decreased body weight, body weight gain	44	100	0.4	1.5

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna for the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 200u9). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
ADBAC (61789-71-7)	Chronic *Daphnia*	0.0042	10	0.00042

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
ADBAC (61789-71-7)	*Chironomus tentans*	520	100	5.2

EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
ADBAC (61789-71-7)	Terrestrial plant toxicity	277	100	2.77

EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

ADBAC is a mixture of discrete benzalkyl quaternary ammonium salts, in the category of unknown or variable composition, complex reaction products or biological materials (UVCBs). Each salt contains an organic cation based on a quaternary nitrogen that is covalently bonded to a benzyl substituent, two methyl groups, and a single alkyl chain that has seven or more carbon atoms. The molecular structure of ADBAC is presented in **Figure 1**.

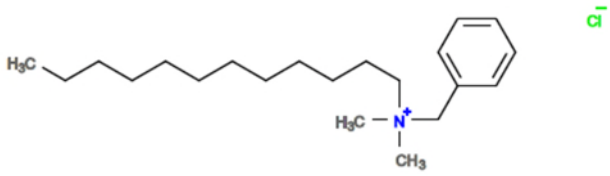

Figure 1 Molecular Structure of ADBAC[2]

This substance is biodegradable and not expected to bioaccumulate. It does have the potential to sorb to soils and settlement. However, sorption is expected to be mitigated by significant biodegradation.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for ADBAC is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that ADBAC is not a PBT substance.

Human Health Hazards

The acute toxicity of ADBAC to humans is relatively moderate by the oral route. The substance is corrosive to skin and is expected to be corrosive to eyes. It is not a sensitiser. In repeat dose toxicity tests, including reproductive studies, NOAELs exceeded 10 mg/kg-day. The substance is not genotoxic nor is it carcinogenic.

Based on a review of a chronic oral toxicity study in rats, toxicological reference values were derived for ADBAC. The drinking water guideline value derived for ADBAC using the non-carcinogenic oral RfD is 1.5 mg/L.

Based on its potential use as a biocide in produced water flow lines, ADBAC may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to ADBAC in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay), and treatment and retention (and associated biodecay) are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of the biocide in produced water would be diluted by a factor of at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a

[2] Source NICNAS, 2016

water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, ADBAC exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the settlement matrix. This substance is not expected to bioaccumulate.

Toxicity data on water, sediment and soil-dwelling organisms was available to calculate PNECs. Experimental results were available for three trophic levels for water and soil organisms. Experimental results were available for one sediment-dwelling organism.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released produced water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at

the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to ADBAC that may occur during water treatment activities. The risk characterisation evaluates the toxicity of ADBAC and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Exposure Point Concentration Calculations

A quantitative mass balance calculation was undertaken to estimate the potential concentrations of contingency water treatment chemicals containing ADBAC within diluted produced water. For the mass balance calculation, Water Management Facility (WMF) process information was used to determine the amount of ADBAC in the water feed pond influent (see **Attachment 2**). **Table 6** presents the estimated pond influent concentration.

Table 6 Mass Balance Estimates for ADBAC

Chemical Name	CAS No.	Water Feed Pond Influent (mg/L)
ADBAC	61789-71-7	7.2E-10

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

The mass balance of ADBAC was then used to estimate potential EPCs for the evaluation of releases of treated water to the Dawson River.

The concentration of ADBAC within the produced water will decrease, where applicable, to account for the biodegradation and photolytic degradation of constituents over time. As a result, the EPC was adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The biodegradation information was obtained from the OECD ready tests (OECD, 1992) that were developed as a first-tier testing scheme to provide preliminary screening of organic chemicals. The ready tests are stringent screening tests that are conducted under aerobic conditions in which a high concentration of the test substance is

used, and biodegradation is measured by non-specific parameters including dissolved organic carbon, biochemical oxygen demand and carbon dioxide production. **Attachment 3, Table 1** includes the environmental fate information that was used to assess biodegradation of the chemical.

The concentrations in the water feed pond were then further reduced by a factor of 99% to account for efficiencies in the WMF system.

Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

These estimated surface water EPCs were used to derive EPCs for sediment using the equilibrium partitioning method. **Attachment 3, Table 1** includes the equation and environmental fate information used to derive the sediment EPC.

Release Scenario Assessment

There is no potentially complete exposure pathway to sources of drinking water; however, as a conservative measure, the theoretical concentrations for the release scenario was compared to human health toxicity-based screening levels to screen for potential effects as a result of surface water used as a drinking water source. The results of this comparison, including the ratio of exceedance of screening levels, is presented in **Attachment 3, Table 2**. As detailed in the table, the risk ratio did not exceed the target level of 1.

To further evaluate potential exposure pathways for aquatic receptors, theoretical concentrations were also compared to the PNECs for aquatic receptors. **Attachment 3, Table 3** presents the results of this comparison, including the ratio of exceedance of screening levels. Similar to above, risk ratios did not exceed the target level of 1.

The primary land use within the development area is agricultural (grazing on improved or unimproved pastures), and it is sparsely populated. To further evaluate potential risks to non-MNES receptors (mammals and avian), additional quantitative analysis of the managed releases to Dawson River was conducted.

Terrestrial receptors evaluated for exposure to Dawson River discharge include domesticated livestock, large mammalian wildlife and small mammalian wildlife. Beef cattle were used to evaluate domesticated livestock, kangaroos were evaluated for large mammalian wildlife, and dingos were evaluated for small mammalian wildlife. The cattle egret was selected to evaluate avian exposures. Exposure assumptions, TRVs and total intake calculations are detailed in **Attachment 3, Tables 4, 5, 6 and 7**. **Attachment 3, Table 4** presents the calculated risk estimates for the kangaroo. **Attachment 3, Table 5** presents the calculated risk estimates for the dingo. **Attachment 3, Table 6** presents the calculated risk estimates for the cattle. **Attachment 3, Table 7** presents the calculated risk estimates for the cattle egret. As indicated in the tables, the calculated HQ for ADBAC did not exceed the risk threshold level of 1 for any of the scenarios evaluated.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 1**), ADBAC does not meet the criteria for persistence or bioaccumulation. It does have the potential to sorb to soils and sediment. However, sorption is expected to be mitigated by significant biodegradation. Further, estimated concentrations in surface water and sediment were less than PNECs. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 7** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 7 Evaluation of Uncertainty – ADBAC

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in water treatment were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	Concentrations of COPCs evaluated in the quantitative risk assessment were assumed to be 100 percent of mass used in the water treatment process. This is a conservative assumption for chemicals that may degrade rapidly or volatilise.	Medium	This assumption may overestimate the calculated risks to receptors.
Exposure Assessment	The use of the food consumption relationship with body weight for mammalian and avian receptors.	Low to Medium	Low to medium potential to underestimate or overestimate risk
Exposure Assessment – EPC	The assessment for all receptors considers the maximum concentration in days 0 and 30 in any one year and does not evaluate further degradation of residual concentrations.	Medium	Medium to high potential to overestimate risks.
Toxicity Assessment	The use of toxicity values in a risk assessment is based on extrapolations from animal data, adjust factors for inherent uncertainty in the toxicological estimate and use of surrogate toxicity criteria	Low	Low potential to underestimate risk
Toxicity Assessment	The use of LOAEL/NOAEL for calculation of the TRVs	Low to Medium	Low to medium potential to underestimate or overestimate risk
Toxicity Assessment	The use of the allometric scaling method to estimate the population-level effects on wildlife based on individual level of exposures.	Low to Medium	Low to medium potential to underestimate or overestimate risk

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Attachment 1 Risk Assessment Dossier

Cocoalkyl dimethylbenzyl ammonium chloride (61789-71-7)

This dossier on cocoalkyl dimethyl benzyl ammonium chloride (ADBAC) presents the most critical studies pertinent to the risk assessment of this substance in its use in drilling muds, hydraulic fracturing fluids and water treatment systems. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from The National Industrial Chemicals Notification and Assessment Scheme (NICNAS, 1994) and the ECHA database that provides information on chemicals that have been registered under the European Union (EU) REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion - ADBAC was not identified in databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. However, ADBAC was assessed as a tier 3 chemical for acute toxicity and as a tier 3 chemical for chronic toxicity. Therefore, ADBAC is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

ADBAC is a mixture of discrete benzalkyl quaternary ammonium salts, in the category of unknown or variable composition, complex reaction products or biological materials (UVCBs). Each salt contains an organic cation based on a quaternary nitrogen that is covalently bonded to a benzyl substituent, two methyl groups, and a single alkyl chain that has seven or more carbon atoms. This substance is biodegradable and not expected to bioaccumulate. It does have the potential to sorb to soils and settlement. However, sorption is expected to be mitigated by significant biodegradation. The acute toxicity of ADBAC to humans is relatively moderate by the oral route. The substance is corrosive to skin and is expected to be corrosive to eyes. It is not a sensitiser. In repeat dose toxicity tests, including reproductive studies, no observed adverse effect levels (NOAEL) exceeded 10 milligrams per kilogram a day (mg/kg-day). The substance is not genotoxic nor is it carcinogenic. ADBAC exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the settlement matrix.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Coco alkyl dimethyl benzyl ammonium chloride

CAS RN: 61789-71-7

Molecular formula: $C_{21}H_{38}ClN$

Molecular weight: 340 g/mol

Synonyms: Alkyl dimethyl benzyl ammonium chloride; Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides; Benzyl (coconut oil alkyl)dimethyl ammonium chloride; Benzyl chloride quaternary salt of N,N'-dimethylcocoamine; Dimethyl cocobenzyl ammonium chloride

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1. This substance as a salt of benzalkyl quaternary ammonium surfactants is expected to have low volatility (de Oude, 1992).

The reported water solubility value is the measured critical micelle concentrations (CMCs) for discrete chemicals in this group (Mukerjee and Mysels, 1971). The CMCs decrease with increasing alkyl chain length as expected (Tezel, 2009).

The octanol-water partition coefficient (K_{ow}) for the chemicals in this group is not considered to provide a reliable indicator of the partitioning behaviour of surface-active substances in the environment (McWilliams and Payne, 2001; Shorts, et al., 2010).

Table 1 Overview of Physico-Chemical Properties of ADBAC[1]

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	White solid	1	ECHA
Melting Point	33°C for transition between solid and paste, and 200°C for transition between paste and liquid	1	ECHA
Boiling Point	218°C	1	ECHA
Density	940 kg/m³	1	ECHA
Vapour Pressure	0 Pa	2	ECHA
Partition Coefficient (log K_{ow})	0.004	2	ECHA
Water Solubility	17 mg/L @ 23°C	1	ECHA
Flash Point	The study does not need to be conducted because the flash point is only relevant to liquids and low melting point solids.	1	ECHA
Auto flammability	No autoignition temperature was observed up to the maximum test temperature of 403°C.	2	ECHA
Viscosity	The study does not need to be conducted because the substance is a solid.	-	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for ADBAC.

[1] 1 Data abstracted from ECHA dossier on quaternary ammonium compounds, benzyl-C16-C18 (even numbered)-alkyldimethyl, chlorides (EC No. 939-290-7) based on structural similarity.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

ADBAC is biodegradable and not expected to bioaccumulate. It does have the potential to sorb to soils and sediment. However, sorption is expected to be mitigated by significant biodegradation.

B. Biodegradation

ADBAC is considered to be readily biodegradable, although no data were provided (EU, 2012). Didecyldimethylammonium chloride (DDAC), a structural analogy of ADBAC, showed 83.3% CO_2 evolution after 28 days in a simulated sewage treatment system. A biodegradation study in two water/sediment systems has been conducted on DDAC. DDAC easily migrated from the aqueous phase to the sediment phase and was easily adsorbed to sediments (high K_{oc}). The degradation in the sediment did not increase very much after the first month and the half-life (DT_{50}) of the total system was not reached within the 120 days test duration (EU, 2012).

C. Environmental Distribution

An OECD Guideline 106 (Adsorption - Desorption Using a Batch Equilibrium Method) was performed based on read-across via grouping to quaternary ammonium salts (ECHA) [Kl. score = 2]. The K_{oc} at 20 degrees Celsius (°C) was determined to be 1.6 $x10^6$ litres per kilogram (L/kg).

D. Bioaccumulation

The measured bioconcentration factor (BCF) in bluegill fish (whole body) after 36 days (35-day exposure plus 21-day depuration) was determined to be 79, with BCF values for edible tissues and non-edible tissues being 33 and 160, respectively (EU, 2012). Thus, ADBAC has a low potential for bioaccumulation (EU, 2012).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

ADBAC disposition in the rat is facilitated by faecal absorption. The acute toxicity is relatively moderate. The substance is corrosive to skin and is expected to be corrosive to eyes. ADBAC is not a sensitiser. In repeat dose toxicity tests, including reproductive studies, NOAEL exceed 10 mg/kg-day. The substance is not genotoxic nor is it carcinogenic.

B. Toxicokinetics

Following a single or repeated oral doses of ADBAC, >90% was excreted in the faeces and 5-8% was eliminated via urine, <1% was present in the tissues seven days after dosing. Thus, it can be assumed that ADBAC is not readily absorbed from the gastrointestinal tract. An oral absorption of 10% can be assumed (EU, 2012).

In an *in vitro* study using human skin, dermal absorption of ADBAC was determined to be 8.3% (EU, 2012).

C. Acute Toxicity

The acute oral LD_{50} values in rats of ADBAC (purity 82.26%) are 510.9 milligrams per kilogram (mg/kg) for males, 280.8 mg/kg for females, and 204.5 mg/kg for both sexes combined (USEPA, 2006a,b) [Kl. score = 2]. The oral LD_{50} in rats is 344 mg/kg (EU, 2012) [Kl. score = 2].

The LC_{50} value of ADBAC (purity 82.26%) is between 0.054 and 0.51 milligrams per litre (mg/L) (USEPA, 2006a,b).

The dermal LD_{50} values of ADBAC (purity 82.26%) in rats are 1,100 mg/kg for males, 704 mg/kg for females, and 930 mg/kg for both sexes combined (USEPA, 2006a,b) [Kl. score = 2]. The dermal LD_{50} in rabbits is 2,848 mg/kg (EU, 2012) [Kl. score = 2].

D. Irritation

ADBAC is corrosive to the skin of rabbits; it is expected to be corrosive to the eyes of rabbits (USEPA, 2006a,b; EU, 2012) [Kl. score = 2].

E. Sensitisation

ADBAC was not a skin sensitiser when evaluated in a guinea pig Buehler test (USEPA, 2006a,b; EU, 2012). Didecyldimethylammonium chloride, a structurally similar compound, was not a skin sensitiser in a guinea pig maximisation test (EU, 2012) [Kl. score = 4].

F. Repeated Dose Toxicity

In sub chronic oral toxicity studies, the NOAELs were 31, 85 and 13.1 mg/kg-day for rats, mice and dogs, respectively. The adverse effects seen in these studies were mainly decreased body weights, reduced feed consumption, and appearance of clinical signs related to the irritation and tissue damage to the gastrointestinal tract. There were changes in the haematological and clinical

chemistry parameters in the high-dose animals that were interpreted as secondary to reduced feed intake and dehydration that led to reduced kidney blood flow (EU, 2012) [Kl. score = 4].

In a chronic oral toxicity study, decreased body weights and body weight gain were observed in rats given 88 mg/kg ADBAC. The NOAEL for the study is 44 mg/kg-day (USEPA, 2006b; EU, 2012) [Kl. score = 2].

In a chronic oral toxicity study, the NOAEL for non-neoplastic effects in mice is 73 mg/kg-day (EU, 2012) [Kl. score = 4].

In a 90-day dermal toxicity study, there were no systemic effects seen at 20 mg/kg-day ADBAC (purity 81.09%), the highest dose that did not elicit excessive skin irritation. The NOAEL is 20 mg/kg-day (USEPA, 2006a; EU, 2012) [Kl. score = 4].

G. Genotoxicity

The *in vitro* genotoxicity studies on ADBAC are presented in Table 3.

Table 3 *In vitro* Genotoxicity Studies on ADBAC

Test System	Results		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains)	-	-	4	USEPA, 2006a; EU, 2012
Mammalian cell gene mutation (CHO cells)	-	-	4	USEPA, 2006a; EU, 2012
Chromosomal aberration (human lymphocytes)	-	-	4	USEPA, 2006a; EU, 2012
Unscheduled DNA synthesis assay	-	Not tested	2	USEPA, 2006a

*+, positive; -, negative

ADBAC was negative in an *in vivo* mouse micronucleus assay (EU, 2012) [Kl. score = 4].

H. Carcinogenicity

ADBAC was not carcinogenic to rats and mice; no details were provided, although the route of exposure is presumed to be oral based on the chronic toxicity study information (USEPA, 2006a; EU, 2012) [Kl. score = 2].

I. Reproductive Toxicity

In a reproductive toxicity study (details not specified), reduced weight gain and feed consumption were noted in the parental and F_1 offspring. The lowest observed adverse effect level (LOAEL) and NOAEL for the parental and F_1 offspring are 100 and 50 mg/kg-day, respectively. The NOAEL for the F_2 offspring is 50 mg/kg-day. There were no reproductive effects at doses that were not maternally toxic (EU, 2012) [Kl. score = 4].

J. Developmental Toxicity

Pregnant female rats were administered ADBAC (route not specified) at doses of 0, 10, 30 or 100 mg/kg (duration not specified). Maternal toxicity was noted at $\geq$ 30 mg/kg; there was no indication of developmental toxicity at any dose level. The NOAEL for maternal toxicity is 10 mg/kg-day; the NOAEL for developmental toxicity is 100 mg/kg-day, the highest dose tested (EU, 2012) [Kl. score = 4].

In a rabbit developmental toxicity study, the NOAEL for maternal toxicity was 3 mg/kg-day. The NOAEL for developmental toxicity was 9 mg/kg-day, the highest dose tested (EU, 2012) [Kl. score = 4].

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for ADBAC follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

For oral exposure, the lowest NOAEL is 44 mg/kg-day from a rat chronic toxicity study based on a LOAEL of 88 mg/kg-day for decreased body weights and body weight gain.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 44/(10 x 10 x 1 x 1 x 1) = 44/100 = 0.4 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.44 x 70 x 0.1)/2 = 1.5 mg/L

L. Human Health Hazard Assessment of Physico-Chemical Properties

ADBAC does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

ADBAC exhibits significant acute and chronic aquatic toxicity. Sediment dwelling organisms are far less sensitive to the substance perhaps based on combined effects of biodegradation and binding to the settlement matrix.

B. Aquatic Toxicity

Table 4 lists the results of acute aquatic toxicity studies on ADBAC.

Table 4 Acute Aquatic Toxicity Studies on ADBAC

Test Species	Endpoint	Results (mg a.i./L)	Klimisch score	Reference
Pimephales promelas	96-hr LC_{50}	0.28	2	USEPA, 2006a; EU, 2012
Daphnia magna	48-hr EC_{50}	0.0058	2	USEPA, 2006a; EU, 2012
Selenastrum capricornutum	72-hr EC_{50}	0.049	2	EU, 2012

a.i. = active ingredient

The chronic aquatic toxicity studies on ADBAC are listed in **Table 2**.

Table 2 Chronic Aquatic Toxicity Studies on ADBAC

Test Species	Endpoint	Results (mg a.i./L)	Kl. score	Reference
Pimephales promelas	24-d NOEC	0.0322	2	USEPA, 2006a,b; EU, 2012
Daphnia magna	21-d NOEC	$\geq$0.00415	2	USEPA, 2006a,b; EU, 2012
Selenastrum capricornutum	EC_{10}	0.009	2	EU, 2012
Lemna gibba	7-d EC_{50}	0.25	2	EU, 2012

C. Sediment Toxicity

The 28-day no observed effect concentration (NOEC) for the midge *Chironomus tentans* is 520 mg/kg dry weight (EU, 2012) [Kl. score = 2].

D. Terrestrial Toxicity

Table 3 lists the results of toxicity studies conducted on ADBAC with earthworms, soil microorganisms and birds.

Table 3 Terrestrial Toxicity Studies on ADBAC

Test Species (method)	Endpoint	Results	Kl. score	Reference
Earthworm *Eisenia fetida*	14-d LC_{50}	7,070 mg/kg soil dw	2	EU, 2012
Mustard plant	18-20-d EC_{50}	277 mg/kg soil dw	2	EU, 2012
Soil microorganisms	28-d EC_{50} 28-d EC_{50}	>1,000 mg/kg soil dw* >1,000 mg/kg soil dw**	2	EU, 2012
Northern bobwhite quail	Acute LC_{50}	164 mg/kg	2	EU, 2012
Northern bobwhite quail	Dietary LC_{50}	>3,813 mg/kg	2	EU, 2012
Mallard duck	Dietary LC_{50}	>2,463 mg/kg	2	EU, 2012

*Nitrogen transformation.
**Carbon transformation.

E. Calculation of Predicted No Effect Concentrations (PNECs)

$PNEC_{water}$: Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (0.28 mg/L), *Daphnia* (0.0058 mg/L) and algae (0.049 mg/L). Results from chronic studies are also available for all three trophic levels, with the lowest NOEC or EC_{10} value being 0.00415 mg/L for invertebrates. On the basis that the data consists of short-term and long-term results from three trophic levels, an assessment factor of 10 has been applied to the lowest reported NOEC of 0.00415 mg/L for invertebrates. The $PNEC_{water}$ is 0.000415 mg/L or 0.415 micrograms per litre (µg/L).

$PNEC_{sediment}$: Experimental results are available for one sediment dwelling organism. In a chronic sediment-spiked test with *Chironomus tentans*, the 28-day NOEC was 520 mg/kg dw. Using an assessment factor of 100, the $PNEC_{sediment}$ was determined to 5.2 mg/kg dw.

$PNEC_{soil}$: Experimental results are available for three trophic levels. Acute EC_{50} values are available for earthworms (7,070 mg/kg dw) and plants (277 mg/kg dw). A long-term study has also been conducted on soil organisms. On the basis that the data consists of acute tests from two trophic levels and a long-term test on one trophic level, an assessment factor of 100 has been applied to the lowest reported EC_{50} value of 277 mg/kg dw for plants. The $PNEC_{soil}$ is 2.8 mg/kg dw.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009).

ADBAC is readily biodegradable; thus, it does not meet the screening criteria for persistence.

The measured BCF for ADBAC is 79; thus, ADBAC does not meet the screening criteria for bioaccumulation.

Chronic NOECs for fish, *Daphnia* and algae are available for ADBAC; the lowest EC_{10} or NOEC value is <0.1 mg/L. Therefore, ADBAC meets the screening criteria for toxicity.

The overall conclusion is that ADBAC is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, ADBAC does meet the criteria for persistence or bioaccumulation. Further evaluation of cumulative impacts is provided in the quantitative risk assessment.

No other characteristics of concern were identified for ADBAC.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cocoalkyl dimethylbenzyl ammonium chloride (ADBAC)	61789-71-7	Not a PBT	No	No	No	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).
3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
µg/L	micrograms per litre
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
CHO	Chinese hamster ovary
COC	constituent of concern
DDAC	didecyldimethylammonium chloride
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
kg/m³	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
mg a.i./L	milligrams active ingredient per litre
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram a day

mg/L	milligrams per litre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	predicted no effect concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	reference dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

Attachment 2 Contingency Biocide Dosing Assumptions

Attachment 2
Summary of Exposure Point Concentration Development
(Contingency Water Treatment Chemicals)

Mass Balance

In other Santos project areas, approximately 413 milligrams per litre (mg/L) of a water treatment product is being dosed (9.2 litres [L] added to approximately 1,380 billion barrels [bbl] or 2.2 x 10^5 litres of legacy/CF1 PFW). The constituent of potential concern (COPC) legacy/CF1 produced formation water (PFW) concentrations are calculated based on the product dose that is apportioned between the COPCs based on the COPC percent weight in the product (composition information in the safety data sheet). The concentration of the COPCs in the water storage pond influent (representative of treatment of combined produced water from legacy/CF1 PFW and bore water) was based on the combined dilution from 2,300 bbl/day.

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	COPC Legacy/CF1 PFW (mg/L)	Storage Pond Influent (mg/L)
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	5	1.0E-04	7.2E-10

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
mg/L = milligrams per litre
PFW = produced formation water

Attachment 3 Risk Characterisation Tables

Attachment 3, Table 1
Summary of Theoretical Biodegradation of Vendor Chemicals in Contingency Water Treatment

Chemical	CAS No.	Estimated Concentration in Water Feed Pond Influent (mg/L)[1]	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF (mg/L)		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[2]		Estimated Concentration in Dawson River Surface Water (mg/L)[3]		Estimated Concentration in Dawson River Sediment (mg/kg)[4]	
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)	
				0	30	0	30	0	30	0	30
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	7.20E-10	1.50E+01	7.20E-10	1.80E-10	7.20E-12	1.80E-12	1.44E-13	3.60E-14	3.46E-09	8.64E-10

Notes:
mg/L = milligrams per liter
mg/kg = milligrams per kilogram
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Water feed pond influent concentrations detailed in Attachment 2.
2) Concentrations in the water feed pond were further reduced by a factor of 99% to account for efficiencies in the WMF system.
3) A dilution factor of 50 was assumed within the approved mixing zone.
4) $EPC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times EPC_{water}$
Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = treated water EPC
$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]
$Kp_{sed} = K_{oc} \times f_{oc}$
Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg), chemical-specific value found in dossier provided in Attachment 1.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

Attachment 3, Table 2
Comparison of Theoretical Concentrations of COPCs to Drinking Water Guidelines
Water Treatment Chemicals

Permeate Pond								
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (mg/L)[1]		Drinking Water Screening Level (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	7.20E-12	1.80E-12	1.44E-13	3.60E-14	1.50E+00	9.6E-14	2.4E-14

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 3, Table 3
Comparison of Theoretical Concentrations of COPCs to PNECs (Water and Sediment)
Water Treatment Chemicals

Permeate Pond													
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (mg/L)[1]		PNEC aquatic (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)		Estimated Concentration in Dawson River Sediment (mg/kg)[1]		PNEC sediment (mg/kg)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30	0	30		0	30
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	7.20E-12	1.80E-12	1.44E-13	3.60E-14	4.20E-04	3.4E-10	8.6E-11	3.46E-09	8.64E-10	3.57E+00	9.7E-10	2.4E-10

Notes:
mg/L = milligrams per liter
mg/kg = milligrams per kilogram
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 3, Table 4
Risk Estimates for Cattle Egret from Vendor Chemicals in Dawson River Release
Water Treatment Chemicals

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Avian NOAELt [1]	Avian NOAEL Test Animal		Avian Receptor Cattle Egret	
			Animal	Body Weight (kg)		Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	4.40E+01	Rat	3.50E-01	NA	Bobwhite Quail	1.78E-01	3.90E-01	4.3E+01

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.03	(c)
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	0.39	Siegfried, 1969
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
W.R. Siegfried (1969) Energy Metabolism of the Cattle Egret, ZoologicaAfricana, 4:2, 265-273, DOI: 10.1080/00445096.1969.11447375
c/ Drinking water ingestion rate (WIR) based on the allometric relationship developed by Calder and Braun (1983), where WIR (L/day) = 0.059 x BW (Kg)$^{0.67}$

Constituent Name	CAS No.	EPC [1] Day 0	EPC [1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/L)	CW (mg/L)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	1.4E-13	3.6E-14	4.3E+01	2.1E-16	5.0E-18	5.3E-17	1.2E-18

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/L = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 3, Table 5
Risk Estimates for Kangaroo from Vendor Chemicals in Dawson River Release
Water Treatment Chemicals

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Mammal Kangaroo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	4.40E+01	Rat	3.50E-01	2.50E+01	6.67E-02

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	3	Fleming, 2001
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	25	Fleming, 2001
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
Fleming, 2001
Fleming, Peter; Laurie Corbett, Robert Harden, Peter Thomson (2001). Managing the Impacts of Dingoes and Other Wild Dogs. Commonwealth of Australia: Bureau of Rural Sciences.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/L)	CW (mg/L)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	1.4E-13	3.6E-14	6.7E-02	3.3E-16	5.0E-15	8.3E-17	1.2E-15

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/L = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 3, Table 6
Risk Estimates for Dingo from Vendor Chemicals in Dawson River Release
Water Treatment Chemicals

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Dingo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	4.40E+01	Rat	3.50E-01	1.30E+01	6.67E-02

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.75	Dawson, 1995
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	13	Dawson, 1995
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
Dawson, 1995
Dawson, Terence J. (1995). Kangaroos: Biology of the Largest Marsupials. Cornell University Press, Ithaca, New York. Second printing: 1998. ISBN 0-8014-8262-3.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/L)	CW (mg/L)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	1.4E-13	3.6E-14	6.7E-02	1.6E-16	2.4E-15	4.0E-17	6.0E-16

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/L = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 3, Table 7
Risk Estimates for Cattle from Vendor Chemicals in Livestock Water
Water Treatment Chemicals

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Cattle	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	4.40E+01	Rat	3.50E-01	4.54E+02	7.33E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weight test}{Body\ Weight receptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	86	API, 2004
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	454	API, 2004
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
API, 2004
API. (2004). Risk-Based Screening Levels for the Protection of Livestock Exposed to Petroleum Hydrocarbons, Regulatory Analysis and Scientific Affairs No. 4733 July 2004.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/L)	CW (mg/L)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Cocoalkyl dimethylbenzyl ammonium chloride	61789-71-7	1.4E-13	3.6E-14	7.3E+00	5.2E-16	7.1E-17	1.3E-16	1.8E-17

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/L = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Qualitative and Quantitative Tier 3 Assessment

Mixture of 5-Chloro-2-Methyl-2H-Isothiazol-3-One and 2-Methyl-2H-Isothiazol-3-One (3:1)

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

The mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) (3:1) is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to improve formation permeability, enhancing the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

The purpose and maximum quantity for this chemical in the total fluid system is summarised in **Table 1**.

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	bactericide	0.00054%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. CMIT/MIT is not a carcinogen, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) (55965-84-9)	2-year rat drinking water	Gastric irritation of the stomach	17	100	0.17	0.60

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicity reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effect concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) (55965-84-9)	Chronic Algae	0.0014	10	0.00014

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) (55965-84-9)	Chronic Oligochaete	0.27	50	0.0054

EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) (55965-84-9)	Soil Microorganisms	1	50	0.02

EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Methylisothiazolinones are made industrially by oxidative cyclisation of the linear organic di-sulfide, N,N'-dimethyl-3,3'-dithiodipropionamide (CAS RN 999-72-4), in a process that uses chlorine as the oxidant. This manufacturing process inevitably produces a mixture of MIT and CMIT, as well as a small amount of the dichloro derivative (DCMIT; CAS RN 26542-23-4). These mixtures are generally not separated into their constituent chemicals and CMIT is not commercially available except as a mixture with MIT (NICNAS, 2020).

The mixture of CMIT and MIT is a powerful biocide and preservative and has a role as an antifouling biocide, an antimicrobial agent, and an antifungal agent. MIT and CMIT use is reported across a wide range of both consumer product uses (e.g. cosmetics, personal care products, baby wipes, automotive and marine sealants and waxes) and industrial uses (e.g. biocides in industrial circulating cooling water systems, preservatives in papermaking, leather treatment and cutting fluids) and are active pharmaceutical ingredients in biological products and prescription medicines (NICNAS, 2000). The molecular structure of the mixture of CMIT and MIT is presented in **Figure 1**.

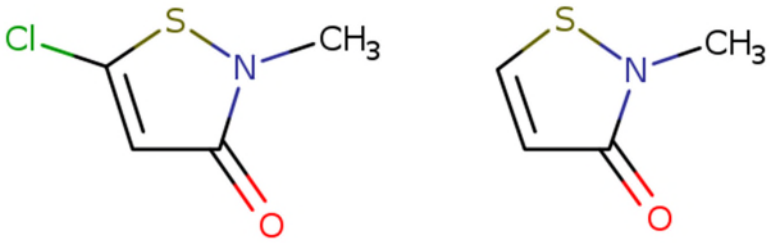

Figure 1 **Molecular Structure of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) with 2-methyl-2h-isothiazol-3-one (MIT)[2]**

Combined formulations of CMIT and MIT are marketed under several trade names, such as Kathon™ 886 and ACTICIDE LG. Magnesium nitrate and magnesium chloride are present in the commercial CMIT/MIT mixture as an inert ingredient and impurity, respectively. The amount of these two salts vary depending on the formulation (EU SCCS, 2009).

The mixture of CMIT and MIT is readily soluble in water and is stable up to pH 9 where extensive degradation is observed. It is susceptible to photodegradation. The mixture of CMIT and MIT is biodegradable at expected environmental exposure concentrations and would also be removed by common biological wastewater treatment facilities. The mixture is not expected to bioaccumulate and has a low potential to adsorb to soil.

The PBT assessment for the mixture of CMIT and MIT is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that CMIT/MIT is not a PBT substance.

[2] Source https://chem.nlm.nih.gov/chemidview/image/55965-84-9?size=3

Human Health Hazards

The acute toxicity of CMIT/MIT is moderate to highly toxic by the oral, inhalation and dermal routes. It is corrosive to the skin and eye and is expected to be a skin sensitiser according to a local lymph node assay.

Repeated exposures to rats by the oral, dermal, or inhalation routes have shown no systemic toxicity; however, evidence of localised irritation (site-of-contact) was observed by all routes of exposure. CMIT/MIT may exhibit weak genotoxic effects in some *in vitro* tests, whereas the *in vivo* studies consistently show no genotoxic activity. It has no reported reproductive or developmental effects; and, is not considered carcinogenic.

A 2-year rat drinking water study has been conducted on a product containing the mixture of CMIT and MIT. The no observed adverse effects level (NOAEL) from this study is 17 milligrams per kilogram-day (mg/kg-day) based on gastric irritation of the stomach. The NOAEL was used to derive the oral RfD and the drinking water guidance value (0.60 mg/L) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

CMIT/MIT may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to CMIT/MIT in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, in the presence of sunlight, CMIT/MIT is susceptible to rapid photodegradation with a half-life of 117 hours, and it is considered rapidly biodegradable in an aerobic aquatic environment with a half-life of 17.3 hours for CMIT and 9.1 hours for MIT in the water/sediment system. Therefore, the biocide is not expected to be a significant risk driver.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

The mixture of CMIT and MIT exhibits significant acute and chronic aquatic toxicity. The mixture is also toxic to sediment dwelling organisms but less toxic to terrestrial receptors. Under expected environmental conditions, the mixture is readily biodegradable and is not expected to bioaccumulate.

PNECs for the mixture of CMIT and MIT are provided in **Tables 3 – 5**. Toxicity data on water, sediment and soil-dwelling organisms was available to calculate PNECs. Experimental results were available for three trophic levels for water and soil organisms. Experimental results were available for one sediment-dwelling organism. PNEC calculations and assumptions are included in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

1. Aquatic ecological receptors within Dawson River downstream of the release point
2. Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released produced water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to the mixture of CMIT and MIT that may occur during hydraulic fracturing and work over activities. The risk characterisation evaluates the toxicity of this chemical and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the EPC by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated and no additional risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Exposure Point Concentration Calculations

A quantitative mass balance calculation was undertaken to estimate the potential concentrations of stimulation chemicals containing CMIT/MIT within diluted produced water. For the mass balance calculation, vendor disclosure forms were used to determine the percentage of CMIT/MIT in the pre-injection fluid. **Table 6** presents the estimated pre-injection fluid concentration.

Table 6 Mass Balance Estimates for CMIT/MIT

Chemical Name	CAS No.	Estimated Pre-injection fluid concentration (mg/L)[1]
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	0.054

1 – Based on volumes provided in Table 1
CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

The mass balance of CMIT/MIT was then used to estimate potential EPCs for the evaluation of releases of treated water to the Dawson River. The potential EPCs have been conservatively estimated.

First, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to the surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no

storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The biodegradation information was obtained from the OECD ready tests (OECD, 1992) that were developed as a first-tier testing scheme to provide preliminary screening of organic chemicals. The ready tests are stringent screening tests that are conducted under aerobic conditions in which a high concentration of the test substance is used, and biodegradation is measured by non-specific parameters including dissolved organic carbon, biochemical oxygen demand and carbon dioxide production. **Attachment 2, Table 1** includes the environmental fate information that was used to assess biodegradation of the chemical.

The concentrations in the water feed pond were then further reduced by a factor of 99% to account for efficiencies in the WMF system.

Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

These estimated surface water EPCs were used to derive EPCs for sediment using the equilibrium partitioning method. **Attachment 2, Table 1** includes the equation and environmental fate information used to derive the sediment EPC.

Release Scenario Assessment

There is no potentially complete exposure pathway to sources of drinking water; however, as a conservative measure, the theoretical concentrations for the release scenarios were compared to human health toxicity-based screening levels to screen for potential effects as a result of a release to surface water used as a drinking water source. The results of this comparison, including the ratio of exceedance of screening levels, is presented in **Attachment 2, Table 2**. As detailed in the table, the risk ratio did not exceed the target level of 1 for any of the scenarios.

Theoretical concentrations were also compared to the PNEC for aquatic receptors. **Attachment 2, Table 3** presents the results of this comparison, including the ratio of exceedance of screening levels. Similar to above, risk ratios did not exceed the target level of 1.

The primary land use within the development area is agricultural (grazing on improved or unimproved pastures), and it is sparsely populated. To further evaluate potential risks to non-MNES receptors (mammals and avian), additional quantitative analysis of the managed releases to Dawson River was conducted.

Terrestrial receptors evaluated for exposure to Dawson River discharge include domesticated livestock, large mammalian wildlife and small mammalian wildlife. Beef cattle were used to evaluate domesticated livestock, kangaroos were evaluated for large mammalian wildlife, and dingos were evaluated for small mammalian wildlife. The cattle egret was selected to evaluate avian exposures. Exposure assumptions, TRVs and total intake calculations are detailed in **Attachment 2, Tables 4, 5, 6 and 7**. **Attachment 2, Table 4** presents the calculated risk estimates for the kangaroo. **Attachment 2, Table 5** presents the calculated risk estimates for the dingo. **Attachment 2, Table 6** presents the calculated risk estimates for the cattle. **Attachment 2, Table 7** presents the calculated risk estimates for the cattle egret. As indicated in the tables, the calculated HQ for CMIT/MIT did not exceed the risk threshold level of 1 for any of the scenarios evaluated.

Cumulative Impacts

The potential for cumulative impacts associated with chemicals used during stimulation activities is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 1**), CMIT/MIT does meet the criteria for persistence or bioaccumulation. Further, estimated concentrations in surface water and sediment were less than PNECs. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health and ecological risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 7** below provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 7 Evaluation of Uncertainty – CMIT/MIT

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in residual stimulation fluids were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Exposure Assessment	The use of the food consumption relationship with body weight for mammalian and avian receptors.	Low to Medium	Low to medium potential to underestimate or overestimate risk

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Toxicity Assessment	The use of toxicity values in a risk assessment is based on extrapolations from animal data, adjust factors for inherent uncertainty in the toxicological estimate and use of surrogate toxicity criteria	Low	Low potential to underestimate risk
Toxicity Assessment	The use of lowest observed adverse effect level (LOAEL)/NOAEL for calculation of the TRVs	Low to Medium	Low to medium potential to underestimate or overestimate risk
Toxicity Assessment	The use of the allometric scaling method to estimate the population-level effects on wildlife based on individual level of exposures.	Low to Medium	Low to medium potential to underestimate or overestimate risk

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Attachment 1 Risk Assessment Dossier

MIXTURE OF 5-CHLORO-2-METHYL-2H-ISOTHIAZOL-3-ONE AND 2-METHYL-2H-ISOTHIAZOL-3-ONE (3:1)
(CAS NO. 55965-84-9)

This dossier on the mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) (3:1) presents the most critical studies pertinent to the risk assessment of the mixture in coal seam gas applications. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – CMIT and MIT were not identified in chemical databases used by NICNAS as an indicator that the chemicals are of concern and are not PBT substances. The mixture of CMIT and MIT were assessed as tier 3 chemicals for acute and chronic aquatic toxicity. Therefore, CMIT/MIT are classified overall as **tier 3** chemicals and require a quantitative risk assessment for end uses.

1 BACKGROUND

The methylisothiazolinones in this assessment belong to a larger group of preservatives and industrial biocides which all have an isothiazolinone heterocyclic ring system. CMIT is the monochloro derivative of parent chemical MIT.

Methylisothiazolinones are made industrially by oxidative cyclisation of the linear organic di-sulfide, N,N’-dimethyl-3,3’-dithiodipropionamide (CAS RN 999-72-4), in a process that uses chlorine as the oxidant. This manufacturing process inevitably produces a mixture of MIT and CMIT, as well as a small amount of the dichloro derivative (DCMIT; CAS RN 26542-23-4). These mixtures are generally not separated into their constituent chemicals and CMIT is not commercially available except as a mixture with MIT (NICNAS, 2020).

The mixture of CMIT and MIT is biodegradable at expected environmental exposure concentrations and would also be removed by common biological wastewater treatment facilities. The mixture is not expected to bioaccumulate, and has a low potential to adsorb to soil.

The acute toxicity of CMIT/MIT is moderate to highly toxic by the oral, inhalation and dermal routes. It is corrosive to the skin and eye and is expected to be a skin sensitiser according to a local lymph node assay. Repeated exposures to rats by the oral, dermal, or inhalation routes have shown no systemic toxicity; however, evidence of localised irritation (site-of-contact) was observed by all routes of exposure. CMIT/MIT may exhibit weak genotoxic effects in some *in vitro* tests, whereas the *in vivo* studies consistently show no genotoxic activity. It has no reported reproductive or developmental effects; and, is not considered carcinogenic.

The mixture of CMIT and MIT exhibits significant acute and chronic aquatic toxicity. The mixture is also toxic to sediment dwelling organisms but less toxic to terrestrial receptors.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Reaction mass of 2-methyl-2H-isothiazol-3-one and 5-chloro-2-methyl-2H-isothiazol-3-one

CAS RN: 55965-84-9

Molecular formula: C_4H_5NOS. C_4H_4ClNOS

Molecular weight: 264.8 g/mol

Synonyms: Bio-Perge; Isothiazolinone chloride; 5-Chloro-2-methyl-4-isothiazolin-3-one -2-methyl-4-isothiazolin-3-one mixture; 3(2H)-Isothiazolone, 5-chloro-2-methyl-, mixt. with 2-methyl -3 (2H) -isothiazolone

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for these substances are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Mixture of CMIT and MIT (3:1)

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Solid, pale yellow to yellow	1	ECHA
Melting Point	22.2°C at 101.3 kPa	1	ECHA
Boiling Point	100.1°C at 101.3 kPa	1	ECHA
Density	1,256 kg/m^3 @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	0.75 @ 27°C	1	ECHA
Water Solubility	3,000 g/L @ 20°C	1	ECHA
Vapour Pressure	2.2 Pa @ 20°C	1	ECHA

Combined formulations of CMIT and MIT are marketed under several trade names, such as Kathon CG, Kathon 886, Kathon 886 WT, Kathon™ 886, ACTICIDE LG, ACTICIDE 14 L, ACTICIDE 14P, Microcare IT, Microcare ITL, etc. (EU SCCS, 2009). Initially, all formulations were prepared as a mixture of two individual active ingredients CMIT and MIT and salts. However, Kathon™ 886 biocide is now defined as a combination of the two active ingredients produced by an integrated production process, resulting in an approximate total of 14% active ingredients, 16% magnesium nitrate, 10% magnesium chloride and 62% water. There is no indication as to when this change was made in the manufacturing process (EU SCCS, 2009).

As such, magnesium nitrate and magnesium chloride are present in the commercial CMIT/MIT mixture as an inert ingredient and impurity, respectively. The amount of these two salts vary depending on the source (EU SCCS, 2009).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for the mixture of CMIT and MIT.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

The mixture of CMIT and MIT is biodegradable at expected environmental exposure concentrations, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Partitioning

The mixture of CMIT and MIT is readily soluble in water. Given low Henry's Law constants for MIT and CMIT (0.005 Pa-m^3/mol and 0.0036 Pa-m^3/mol, respectively), these chemicals are considered slightly volatile from water and moist soil. The mixture is also expected to volatilise from dry soil surfaces based upon its vapour pressure.

Based on hydrolysis measurements made using OECD Guideline 111, CMIT/MIT was stable (<10% degradation) at pH 4 and 7. At pH 9 extensive degradation of CIT/MIT was observed. The rate constant was found to be 0.0283 per day and the DT50 and DT90 to be 24.5 days and 81 days, respectively (ECHA). [Kl. Score = 1].

In the presence of sunlight, CMIT/MIT is susceptible to rapid photodegradation with DT50 and DT90 values of 117 and 389 hours, respectively. (ECHA). [Kl. Score = 1].

C. Biodegradation

The biodegradation of the test substance, a 14% aqueous solution of 3 parts 5 -Chloro-2 -methyl-2H-isothiazol-3 -one and 1 part 2 -Methyl-2H-isothiazol-3 -one (cited as ACTICIDE® 14 in the study report), was investigated in a closed-bottle seawater test according to OECD guideline 306. The test substance was incubated with natural seawater over a period of 28 days under aerobic conditions, and oxygen content was determined by means of an oxygen electrode after 0, 5, 15 and 28 days.

ACTICIDE® 14 can be considered inhibitory to bacteria in the seawater sample. Due to inhibition of bacteria, the biodegradability of ACTICIDE® 14 could not be established in this test (ECHA). [Kl. Score = 1].

Biodegradation studies on CMIT and MIT separately have also been conducted. In these studies, CMIT is classified as being readily biodegradable, failing the 10 -day window and MIT is classified as being not readily biodegradable according to the criteria of the test, although significant biodegradation occurred (ECHA).

An OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) was performed on MIT. 50% of the test substance biodegraded within 29 days. Although extensive metabolism occurs over the 29-day interval, the test material does not meet the requirements for readily biodegradable but can be considered ultimately biodegradable. [Kl Score=1](ECHA). The same test with CMIT showed up to 62% of the test substance biodegraded within the same time frame of 29 days. [Kl Score=1](ECHA). The rate of biodegradation in these tests does not satisfy the OECD criterion for readily biodegradability (60% in a 10-day window), but the results do show that these chemicals are biodegradable at more realistic environmental exposure concentrations (NICNAS, 2020).

The primary aerobic biodegradability of MIT has been examined in a river sediment-water system by use of a 14C-labelled model compound. During the 7-day experiment 14C-labelled MIT was rapidly metabolized as only 12.6% of the initial MIT was present after 24 hours of incubation at 25C. The calculated half-life for the parent compound was 9.1 hours (Reynolds, 1994a). The primary biodegradability of CMIT has been examined with the same type of sediment and water as described for MIT. The 14C-labelled CMIT was rapidly metabolized as only 30% of the initial CMI remained after 24 hours of incubation at 25°C. The calculated half-life for the intact CMIT was 17.3 hours (Reynolds, 1994b).

In soil, CMIT and MIT are rapidly biodegradable with reported half-lives of 10.4 hours and 6.5 hours, respectively (ECHA). [Kl. Score = 1].

If a chemical is found to be readily or inherently biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

An OECD Guideline 106 (Adsorption - Desorption Using a Batch Equilibrium Method) was conducted on the CMIT/MIT mixture. The adsorption/desorption characteristics of [14C]-CMIT/MIT were studied in two UK sewage sludges; Basildon (pH 6.6, 29.3% organic carbon) and Chelmsford (pH 6.7, 23.7% organic carbon) and three UK soils, Farditch silt loam (pH 5.5, 4.19% organic carbon), Longwoods sandy loam (pH 7.1, 1.62% organic carbon) and Kenslow loam (pH 4.9, 3.88% organic carbon) using the batch equilibrium method. The Kfoc values obtained ranged from 34 to 54 mL/g (mean of 44 mL/g). The Freundlich exponents (1/n) ranged from 0.564 to 0.778, indicating a non-linear relationship between adsorption and concentration with a higher degree of adsorption to soil at lower concentrations. The determined Kfoc values indicated that CMIT/MIT can be classified as being of intermediate to high mobility in soil. [Kl Score=1](ECHA).

Soil adsorption coefficients (K_{oc}) for MIT (log K_{oc} = 1.08) and CMIT (log K_{oc} – 1.28) indicate both chemicals will have very high mobility in soil (NICNAS, 2020). Likewise, if released to water, based on their high solubility, they are not expected to adsorb to suspended solids or sediments.

E. Bioaccumulation

Bioaccumulation studies are not available for the CMIT/MIT mixture. Individually, MIT and CMIT are not expected to bioaccumulate. Studies of the bioconcentration of MIT and CMIT in bluegill sunfish (Lepomis macrochirus) at an exposure concentration of 0.12 mg/L showed bioconcentration factors (BCF) in this species of 2.3 and 114 L/kg respectively (Madsen, et al., 2001).

The low bioconcentration potential, hydrophilicity, and the reactivity of both chemicals with biomolecules indicate that they will not biomagnify in aquatic or terrestrial food webs (NICNAS, 2020).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

The acute toxicity of CMIT/MIT is moderate to highly toxic by the oral, inhalation and dermal routes. It is corrosive to the skin and eye and is expected to be a skin sensitiser according to a local lymph node assay. Repeated exposures to rats by the oral, dermal, or inhalation routes have shown no systemic toxicity; however, evidence of localised irritation (site-of-contact) was observed by all routes of exposure. CMIT/MIT may exhibit weak genotoxic effects in some *in vitro* tests, whereas the *in vivo* studies consistently show no genotoxic activity. It has no reported reproductive or developmental effects; and, is not considered carcinogenic.

B. Toxicokinetics and Metabolism

Rats were given by gavage a single dose of 3.75 milligrams per kilogram body weight (mg/kg bw), 11.25 mg/kg bw or 22.5 mg/kg bw radiolabeled CMIT. CMIT was rapidly and extensively excreted in the urine and faeces following oral administration. A majority of the radioactivity was excreted from the rats in 24 hour (77-87%). Renal and fecal routes of elimination were equally important. Tissues contained 0.93-1.44% (female and male, respectively) of dosed radioactivity in the low dose group and 3.94-4.72% (female and male, respectively) in the high dose group. The highest amount of radioactivity was found in blood, particularly in red blood cells (0.67-1.09% of the dose in the low dose group, and 3.41-4.11% in the high dose group), followed by muscle (0.15%) in low dose group, and by muscle and liver (0.25%) in high dose group. Gender differences in excretion appeared to be minimal. CMIT was extensively metabolized. Approximately twenty-nine radioactive components were observed in urine and faeces samples from the HPLC radio profiling. Among these N-methyl malonamic acid was detected as the major component in the urine (15.35-18.19%). 3 -mercapturic acid conjugate of 3 -sulfinyl-N-methyl-propionamide was detected as the major component in the feces (up to 32.54%). All other metabolites accounted for less than 5% of the dose. Metabolites are thought to result from reduction and oxidation reactions involving phase I enzymes followed by conjugation to glutathione, giving rise to conjugates to glutathione or to mercapturic acid. (ECHA). [Kl. Score = 1].

C. Acute Toxicity

<u>Oral</u>

An acute oral toxicity study was conducted in 1977 before implementation of the GLP. Groups of CD rats were administered orally via gavage Kathon 886 at 221, 313, 442, 625 or 883 mg/kg b.w. Clinical

signs were observed in all dose levels of this study. Under the conditions of the study, the acute oral LD_{50} in male rats is based on the lowest value, 457 mg/kg Kathon 886 corresponding to 64 mg/kg active ingredient (a.i.) (pure CMIT/MIT). (ECHA). [KI Score = 2].

Inhalation

An acute inhalation toxicity study was conducted in accordance with GLP and as per OECD 403 guideline. Groups of male and female CD (BR) rats were exposed to an aerosol of Kathon 886 via nose only at concentrations of 0.19, 0.32, 0.50, 1.26, 2.24, and 3.02 mg test material/L. Signs of respiratory irritation, including gasping, rales, hyperpnea, dyspnea and vocalization, were seen in some animals in all groups immediately post-exposure. The number of animals showing these signs and the severity of the respiratory irritation correlated with the concentration of the test material to which the animals were exposed in the report. The signs of respiratory irritation disappeared in all surviving animals, taking from two to twelve days. Under the conditions of the study, a combined male and female LC_{50} value of 0.33 mg a.i per litre of air was determined (ECHA). [KI Score = 1].

Dermal

An acute dermal toxicity study was conducted in 1976 before implementation of the GLP. Male albino rabbits were exposed dermally to Kathon 886 at 313, 625, 1250 and 2500 mg/kg under occlusive conditions. Skin irritation consisted of severe erythema and edema followed by eschar formation. LD_{50} was determined to be 660 mg Kathon^{TM} 886/kg bw with 95% confidence limits of 370 and 1210 mg/kg. This corresponds to LD_{50} = 87.12 mg/kg a.i. (pure CMIT/MIT). (ECHA). [KI Score = 2].

D. Irritation

Skin

Two OECD 404 guideline compliant studies are provided indicating CMIT/MIT is corrosive to the skin.

A skin irritation/corrosion study was conducted according to OECD Guideline 404. As part of the study, white rabbits under semiocclusive conditions were exposed to the test substance for 1 or 4 hours. A severe edema (score = 4) was observed in five animals and one animal had a moderate edema (score = 3) one hour after patch removal. This edema was raised more than 2 mm and extended beyond the area of exposure. By day 3, this irritation reversed such that only 3 animals had a slight edema. There was total recovery after 8 days. One animal had a well-defined erythema with slight eschar formations. A reversal was observed after 72 h with total recovery after 11 days. Under the conditions of the study, the material was classified as corrosive to skin following a 1-hour or 4-hour exposure period, but the effects were fully reversible [KI. Score = 2](ECHA).

A second skin irritation/corrosion study was also conducted according to the OECD Guideline 404. In the study, the irritating or corrosive potential of a 13.9 % aqueous solution of a 3:1 mixture of 5 -chloro-2 -methyl-2H-isothiazol-3 -one and 2 -methyl-2H-isothiazol-3 -one in water (named ACTICIDE 14 in this study report) was evaluated. One male New Zealand White rabbit was treated by on the exposed skin with 0.5 ml of the test item for 4 hours. The test substance was removed, and the treated skin was observed for abnormalities, their severity and eventual reversibility. Findings were scored according to the system proposed by Draize. Severe erythema and edema were observed

shortly after treatment. While erythema was not reversible, edema was not observed after day 7. (ECHA). [Kl. Score = 1].

Eye

An in vivo eye irritation study indicated that Kathon™ 886 produces severe lesion to the eyes of rabbit which were not reversible. Kathon™ 886 should be considered as corrosive to the eyes of rabbits. (ECHA). [Kl. Score = 2].

E. Sensitisation

A local lymph node assay (LLNA) study in CBA/J mice was conducted in compliance with the proposed Local Lymph Node Assay protocol prepared by the Interagency Coordinating Committee for Validation of Alternative Methods (ICCVAM) Immunotoxicology Working Group (IWG): National Institutes of Health Publication N°: 99-449, Appendix J, 1999. Groups of mice were exposed to Kathon 886 at nominal concentrations of 0, 30, 50, 70, 90, 360, 1000 ppm a.i. in 4:1 acetone/olive oil and evaluated for skin sensitisation reactions. All concentrations evaluated produced a stimulation index greater than or equal to 3. The results of the study indicate that the test material CMIT/MIT exhibits a statistically significant, generally dose-related potential to induce contact hypersensitivity in mice. [Kl Score=1] (ECHA).

The potential of a 14% aqueous solution of 3 parts 5 -chloro-2 -methyl-2H-isothiazol-3 -one and 1 part 2 -methyl-2H-isothiazol-3 -one (ACTICIDE 14) to cause skin sensitisation was investigated in a Guinea Pig Maximisation Test according to OECD guideline 406. Male and female Dunkin-Hartley guinea pigs were treated with the test substance by intradermal injection (mixed with Freud`s complete Adjuvant) and 6 days later by cutaneous application under occlusive dressing for 48 hours (induction). Two weeks later, animals were treated with the test substance by cutaneous application for 24 hours at a site different from the first application sites (challenge). After another week, animals of the low-dose group were treated with the test substance by dermal application at a lower dose (rechallenge). Slight to moderate erythema were observed after intradermal induction, and local irritation after cutaneous induction. At challenge, all substance-induced animals and half of the control animals presented signs of severe skin reactions. Therefore, animals of the low dose group and a new control group were re-challenged one week later with 100 -1000 -fold less substance by dermal route. In the rechallenge, only animals treated with the high concentration (0.025% ACTICIDE 14) responded positive (4 of ten animals), while animals treated with factor ten lower amounts and the control animals showed no signs of toxicity. [Kl Score = 1](ECHA).

F. Repeated Dose Toxicity

Oral

CMIT/MIT was tested in several oral repeated dose toxicity studies in rabbits, rats and dogs for 4 weeks and 3 months.

The toxic potential of a 13.9 % aqueous solution of a 3:1 mixture of 5 -chloro-2 -methyl-2H-isothiazol-3 -one and 2 -methyl-2H-isothiazol-3 -one in water (ACTICIDE 14) was evaluated in a 90-day repeated dose dietary toxicity study in non-rodents according to OECD guideline 409. Male and female beagle dogs were treated with the test item by dietary administration over a period of 90 days. The animals were observed for clinical signs, alterations in body weight and food consumption

throughout the study period. At selected timepoints before and during the study, blood was collected for haematology and clinical chemistry. At the end of the treatment period, the animals were sacrificed and subjected to detailed macroscopic and microscopic pathological examination.

A dose-dependent loss of bodyweight and reduction in food consumption was observed, while all other observed alterations/abnormalities could not be related to treatment and were considered incidental. The applied doses could analytically not be verified, and thus the exposure doses of the test animals were calculated from the worst-case recovered values.

The observed effects on body weight gain were only seen at the two highest doses and were probably the result of the poor palatability of the diet rather than any toxic properties of ACTICIDE 14. Thus, it was concluded that there was no evidence of organ or systemic toxicity when ACTICIDE 14 was offered in the diet at an analysed dose level up to 555 ppm (nominal concentration 750 ppm) which is equivalent to 22 mg ai/kg body weight/day (30 mg ai/kg body weight/day) to the laboratory beagle for up to 13 weeks. A No Observed Adverse Effect Level (NOAEL) of 22 mg/kg bw/day was established. (ECHA). [Kl. Score = 1].

In a repeated dose 90-day oral toxicity study in rodents, no systemic toxic effects and no adverse effects on the histopathology of any tissues/organs distant from the site of dosing (drinking water) was observed. A NOAEL of 250 ppm ai in water (16.3 mg a.i./kg/day in males and 24.7 mg a.i./kg/day in females) was established. (ECHA). [Kl. Score = 1].

In another oral toxicity study, administration of Kathon™ biocide to male and female rats in the drinking water for 24 months at concentrations up to and including 300 ppm a.i. showed no effects on the type or incidence of neoplasms in any group. No systemic effects were observed. Treatment-related morphologic changes were observed only in the stomach of both sexes in mid and high dose groups. Gastric irritation was the primary effect observed. No adverse effects on the histopathology of any tissues/organs distant from the site of dosing. Based on the study findings, a NOAEL of 300 ppm was established (17.2 mg a.i./kg bw/day in males and 25.7 mg a.i./kg bw/day in females). (ECHA). [Kl. Score = 1].

Inhalation

In a 90-day sub-chronic inhalation study, conducted in accordance with GLP and as per OECD 403 guideline, groups of male and female CD (SD) BR rats were exposed to an aerosol of Kathon 886 via nose only at concentrations of 0.34, 1.15 and 2.64 mg/m^3. There were no systemic effects in this study. Rats at the highest dose (2.64 mg/m^3) exhibited very mild, low grade respiratory irritation. No adverse effects on the histopathology of any tissues/organs distant from the site of dosing. A NOAEL of 0.34 mg/m^3 was established. (ECHA). [Kl. Score = 1].

Dermal

The toxic potential of a 13.9 % aqueous solution of a 3:1 mixture of 5 -chloro-2 -methyl-2H-isothiazol-3 -one and 2 -methyl-2H-isothiazol-3 -one in water (ACTICID 14) was evaluated in a 90-day repeated dose dermal toxicity study in rats according to EPA OPP 82 -3 guideline. Male and female Sprague-Dawley rats were treated with the test item on exposed skin daily for 6 hours over a period of 90 days. The test article was kept in place and prevented from oral ingestion by means of a semi-occlusive dressing for exposure and remainders of the test item were then removed with water. The animals were observed for mortality, clinical signs, body weight gain and food consumption. At the

end of the treatment period, blood and urine were collected for haematology and clinical chemistry. The animals were subjected to detailed macroscopic and microscopic pathological evaluation, including scoring of observed skin abnormalities.

Mortalities observed in two control animals and one high-dose male are considered to be incidental and not related to the application of the test material. Treatment with the test article ACTICIDE 14 applied dermally to intact skin produced skin reactions (slight to moderate erythema and desquamation, slight edema and atonia as well as eschar formation) with dose-dependent grades of severity. Females appeared to be more sensitive than males. There were no other effects at the end of the treatment period that could be attributed to the test substance. A NOAEL for systemic toxicity was established as 2.625 mg a.i. /kg bw/day. A NOAEL for local irritation was established as 0.105 mg a.i./kg bw/day in males. No NOAEL for local irritation was established for female rats. (ECHA). [Kl. Score = 1].

A 90-day subchronic dermal toxicity study was conducted in White New Zealand Rabbits. Doses of 100, 200 and 400 ppm of Kathon 886 were applied 5 days per week for a minimum total of 65 applications. Slight to severe erythema and slight edema were noted in a dose-related manner (0.1 mg/kg/day and above). There were no systemic effects in this study. No adverse effects on the histopathology of any tissues/organs distant from the site of dosing. A NOAEL of 400 ppm a.i. based on skin irritation (0.4 mg/kg bw/day) was established. (ECHA). [Kl. Score = 2].

G. Genotoxicity

In Vitro Studies

Several in vitro studies of genotoxicity were performed with CMIT/MIT. Positive results were observed in three Ames assays and in three tests in mammalian cells (one chromosomal aberration test and two mouse lymphoma assays), with or without S9 activation. (ECHA).[Kl. Score =1 or Kl. Score =2]. In contrast, CMIT/MIT was not mutagenic in primary culture of rat hepatocytes [Unscheduled DNA Synthesis (UDS)] and in a mouse cell transformation test.(ECHA) [Kl. Score =1 or Kl. Score = 2].

In Vivo Studies

CMIT/MIT was tested in one in vivo chromosomal aberration assay in mice (bone marrow) and one micronucleus test in mice (bone marrow). Negative results were observed in these in vivo studies. (ECHA). [Kl. Score = 1].

In the absence of genotoxicity, additional tests were carried out in tissue other than bone marrow. Two UDS assays in rats confirmed the absence of genotoxicity of CMIT/MIT when tested in vivo. (ECHA). [Kl. Score = 1].

H. Carcinogenicity

Oral

An OECD Guideline 453 (Combined Chronic Toxicity / Carcinogenicity Studies) on male and female Crl:CD BR rats was performed. Administration of the substance to male and female rats in the drinking water for 24 months at concentrations up to and including 300 ppm a.i. (17.2 mg a.i./kg of

body weight/day in males and 25.7 mg a.i./kg of body weight/day in females) showed no effects on the type or incidence of neoplasms in any group.

No treatment-related signs of toxicity were seen at 30 ppm a.i.(2.0 mg a.i./kg of body weight/day in males and 3.1 mg a.i./kg of body weight/day in females), the No-Observed Effect Level (NOEL) in this study [Kl Score = 1](ECHA).

Dermal

The mouse skin painting carcinogenicity study was initiated prior to the adoption of carcinogenicity study guidelines. However, the principles of OECD Guideline 451, in general, were followed. Kathon™CG, when applied dermally to the closely clipped skin on the backs of male CD-1 mice at a concentration of 400 ppm active substance and at a dose of 25 microliters (µL) 3 times per week for 30 months, showed no local or systemic tumorigenic potential. No adverse effects were seen on the histopathology of any tissues/organs distant from the site of dosing. (ECHA). [Kl. Score = 2].

I. Reproductive/Developmental Toxicity

An OECD Guideline 416 (Two-Generation Reproduction Toxicity Study) was performed on male and female Sprague-Dawley rats exposed to Kathon™ 886F biocide in the drinking water. No treatment-related deaths or clinical signs of systemic toxicity in either sex up to and including 300 ppm. No treatment-related effects on body weights up to and including 100 ppm in males and females and 300 ppm in females. In 300 ppm males, a treatment-related decrease (5 %) in mean body weight was seen during weeks 1 through 6 of treatment. No treatment-related effects on premating feed consumption in either sex at any dose level. Treatment-related and concentration-dependent decreases in water consumption were noted in all-Kathon™ exposed groups in both the P1 and P2 animals through most of the premating, gestation and lactation periods. No treatment-related effects on any endpoint of mating or fertility in either generation at any dose level. No treatment related effects on sperm motility, testicular sperm count or caudal epididymal reserves of P1 and P2 males at any dose level. Treatment-related microscopic findings were limited to the stomach of male and female parental animals at 100 and/or 300 ppm. These changes included an increased incidence of focal superficial erosions of the glandular mucosa, edema and inflammation of the submucosa of the glandular and nonglandular areas, and hyperplasia and hyperkeratosis of the nonglandular stomach. Based on these findings, a NOAEL for parental animal toxicity of 30 ppm (2.8-4.4 mg/kg/day in the P1 animals and 4.3-5.5 mg/kg/day in the P2 animals) was established. The reproductive and developmental NOEL was 300 ppm (22.7-28.0 mg/kg/day in the P1 animals and 35.7-39.1 mg/kg/day in the P2 animals).(ECHA). [Kl. score = 1]

An OECD Guideline 415 (One-Generation Reproduction Toxicity Study) was performed on male and female Sprague-Dawley rats exposed to Kathon™ 886F biocide in the drinking water. Kathon™ 886 NAR has no adverse effects on the reproductive capability of male or female rats and no effect on fetal health or survival to day 21 at concentrations up to and including 225 ppm in the drinking water. These values correspond to a dose level of 16.3 mg/kg/day in males and 24.7 mg/kg/day in females. (ECHA). [Kl. score = 1]

The potential of a 14% aqueous solution of 3 parts 5 -chloro- 2 -methyl-2H-isothiazol-3 -one (CMIT) and 1 part 2 -methyl-2H-isothiazol-3 -one (MIT) (ACTICIDE 14) to induce teratogenic effects in rats was evaluated in a Prenatal Developmental Toxicity Study (according to guideline EPA OPP 83 -3). Pregnant female Sprague-Dawley rats were treated with the test substance by oral gavage during

the period of organogenesis (days 6 -15 post coitum). Animals were observed for mortality, signs of toxicity, food consumption and body weight gain during the treatment and a post-exposure period of 5 days. At day 20 of gestation, animals were sacrificed and examined for macroscopic pathological abnormalities. Uterine contents were examined for signs abnormal pregnancy courses, and fetuses were examined for external, visceral and skeletal abnormalities.

Treatment with the test article resulted in maternal toxicity with clearly distinguished dose-dependent grades of severity (clinical signs, moderately reduced body weight gain, slightly reduced food consumption). In spite of the observed adverse maternal effects, treatment with the test article did not have any influence on the embryonic and fetal development, as there was no embryotoxicity and no teratogenicity detected in any of the dose groups. (ECHA). [Kl. Score = 1].

An equivalent OECD Guideline 414 (Prenatal Developmental Toxicity Study) was performed on male and female Sprague-Dawley rats exposed to Kathon™ 886F biocide administered orally by gavage. No developmental effects were observed. Kathon™ 886 is non-teratogenic to the rat when administered at dosages of 100 mg/kg/day (15 mg ai/kg bw/day) during organogenesis. (ECHA). [Kl. Score = 1].

An OECD Guideline 414 (Prenatal Developmental Toxicity Study) was performed on pregnant New Zealand white rabbits exposed to Kathon™ 886 MW Biocide administered orally by gavage. No treatment-related deaths were observed at doses of 0, 0.5, 2 or 8 mg a.i./kg. At 20 mg a.i./kg, 16/16 animals were sacrificed moribund on or before day 15 G. Based on the results of this study, a maternal NOEL of 2 mg a.i./kg and an embryo-fetal NOEL of 8 mg a.i./kg was established. No treatment related increases were detected in the type or incidence of external, visceral or skeletal malformations, variations due to retarded development or in the total of these two categories combined. (ECHA). [Kl. Score = 1].

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

Toxicological reference values were derived for the mixture of CMIT and MIT using methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011) as shown below.

Non-Cancer

A two-year drinking water study has been conducted in rats with a CMIT/MIT mixture (14.2% a.i.; 10.13% CMI/3.85% MI). No systemic toxicity was observed at doses up to 300 ppm a.i., although there was gastric irritation of the stomach at doses of 100 and 300 ppm a.i. The NOAEL for systemic toxicity in this study is 300 ppm (corresponding to 17.2 mg a.i./kg bw/day in males and 25.7 mg a.i./kg bw/day in females). The lowest NOAEL from this study (17 mg/kg bw/day) will be used to derive the oral reference dose.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10

UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 17.2/(10 x 10 x 1 x 1 x 1) = 17.2/100 = 0.17 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD:

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.17 x 70 x 0.1)/2 = 0.60 mg/L

Cancer

The mixture of CMIT and MIT was not carcinogenic to rats in a two-year dietary study. Thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

CMIT/MIT does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The mixture of CMIT and MIT exhibits significant acute and chronic aquatic toxicity. The mixture is also toxic to sediment dwelling organisms but less toxic to terrestrial receptors.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on the mixture of CMIT and MIT.

Table 3 Acute Aquatic Toxicity Studies on CMIT/MIT

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Rainbow Trout (*Oncorhynchus mykiss*)	96-hour LC_{50}	0.19	1	ECHA
Water Flea *(Daphnia magna)*	48-hour EC_{50}	0.16	1	ECHA
Skeletonema costatum	72-hour EC_{50} growth rate	0.0063	1	ECHA
Selenastrum capricornutum	72-hour EC_{50} growth rate	0.0273	1	ECHA

Chronic Studies for MIT/CMIT

Table 4 lists the results of chronic aquatic toxicity studies conducted on the mixture of CMIT and MIT.

Table 4 Chronic Aquatic Toxicity Studies on CMIT/MIT

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Rainbow Trout (*Oncorhynchus mykiss*)	38-day NOEC	0.02	1	ECHA
Water Flea *(Daphnia magna)*	21-day NOEC	0.10	1	ECHA
Skeletonema costatum	72-hour NOEC	0.0014	1	ECHA

C. Sediment Toxicity

The 28-day no observed effect concentration (NOEC) for Oligochaete (*Lumbriculus variegatus*) is 0.27 mg/kg dry weight based on survival (ECHA) [Kl. score = 2].

The 28-day no observed effect concentration (NOEC) for the midge *Chironomus riparius* is 3.65 mg/kg dry weight based on survival (ECHA) [Kl. score = 1].

D. Terrestrial Toxicity

An OECD Guideline 208 (Terrestrial Plants Test: Seedling Emergence and Seedling Growth Test) was conducted on CMIT/MIT. No apparent signs of treatment-related phytotoxicity was observed to any of the three species tested (Trifolium pratense, Oryza sativa and Brassica napus). A 21-day NOEC of 1000 mg/kg soil dw, the highest concentration tested, was derived from the study results (ECHA). [Kl. Score = 1].

Effects on soil microflora carbon respiration transformation (OECD Guideline 217) and effects on nitrogen transformation activity of soil microorganisms (OECD Guideline 216) was also studied. Greater than 50 % respiration rate inhibition was demonstrated at test concentrations of 50, 100 and 500 mg CMIT/MIT per kg dry weight soil. A 28-day NOEC value of 1 mg/kg soil dw (based on respiration rate) was determined. (ECHA) [Kl. Score = 1]. CMIT/MIT inhibited the nitrogen

transformation process in active soil within the range of concentrations evaluated. A 28-day NOEC value of 10 mg/kg soil dw (based on nitrate formation rate) was determined. (ECHA) [Kl. Score = 1]..

An acute toxicity test with the earthworm *Eisenia fetida* under static conditions in artificial soil was performed with ACTICIDE® 14 (14.3% aqueous solution of CIT and MIT (3:1)) according to OECD Guideline 207 and ISO 11 268-1. Five concentrations were tested ranging from 100 to 1000 mg ACTICIDE® 14/kg dry soil (nominal). ACTICIDE® 14 caused clear sub-lethal but only moderate lethal effects in earthworms. A NOEC of 100 mg/kg dry soil (=14.3 mg a.i./kg dry soil) due to reduced mobility of the worms and a 14-day LC_{50} of >1000 mg/kg dry soil (>143 mg a.i./kg dry soil) was determined. (ECHA). [Kl. Score = 1].

Results from toxicity studies on mallard duck (*Anas platyrhynchos*) and bobwhite quail (*Colinus virginianus*) demonstrate that C(M)IT/MIT exhibits slight to moderate toxicity to birds. The 21-day oral LD_{50} for bobwhite quail is 64.5 mg/kg bw. The short-term (8-day) dietary LC_{50} for mallard duck is 945 mg/kg and bobwhite quail is 3532 mg/kg (ECHA). [Kl. Score = 1].

E. Calculation of PNEC

The PNEC calculations for CMIT/MIT follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (0.19 mg/L), invertebrates (0.16 mg/L) and algae (0.0063 mg/L). Results from chronic studies are also available for all three trophic levels, with the lowest NOEC value being 0.0014 mg/L for algae. On the basis that the data consists of short-term and long-term results from three trophic levels, an assessment factor of 10 has been applied to the lowest reported NOEC of 0.0014 mg/L for algae. The $PNEC_{water}$ for CMIT/MIT is 0.00014 mg/L.

PNEC sediment

Experimental results are available for two sediment dwelling organisms. The lowest NOEC was observed in a chronic sediment-spiked test with Oligochaete, the 28-day NOEC was 0.27 mg/kg dw. Using an assessment factor of 50, the $PNEC_{sediment}$ was determined to 0.0054 mg/kg dw.

PNEC soil

Experimental results are available for three trophic levels. Acute $E(L)C_{50}$ values are available for earthworms (>1000 mg/kg dw). Long-term studies have also been conducted on plants and soil microorganisms. On the basis that the data consists of acute tests from one trophic level and long-term tests from two trophic levels, an assessment factor of 50 has been applied to the lowest reported NOEC value of 1 mg/kg dw for soil microorganisms. The $PNEC_{soil}$ is 0.02 mg/kg dw.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2017).

The biodegradability of the mixture of CMIT and MIT could not be established. Biodegradation studies on CMIT and MIT separately have been conducted. An OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) was performed. 50% of the MIT biodegraded within 29 days. While the substance does not qualify as readily biodegradable, the data suggest it is ultimately biodegradable. The same test with CMIT showed up to 62% of the test substance biodegraded within the same time frame of 29 days. [KI Score=1](ECHA). The rate of biodegradation in these tests does not satisfy the OECD criterion for readily biodegradability (60% in a 10-day window), but the results do show that these chemicals are biodegradable at more realistic environmental exposure concentrations. Thus, CMIT/MIT do not meet the criteria for persistence.

Bioaccumulation studies are not available for the CMIT/MIT mixture. Individually, the experimental BCF for CMIT is 67-114 in bluefish sunfish, and the BCF for MIT was determined to be 2.3. Thus, CMIT/MIT do not meet the criteria for bioaccumulation.

The chronic toxicity data on the mixture of CMIT and MIT has a NOEC < 0.1 mg/L.. The lowest acute LC_{50} value for the mixture are < 1 mg/L. Therefore, CMIT/MIT meets the criteria for toxicity.

The overall conclusion is that the mixture of CMIT/MIT is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioaccumulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, both CMIT/MIT mixture do not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for the mixture of CMIT and MIT.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	Not a PBT	No	No	No	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

CAS No. = chemical abstracts service number

COC = chemical of concern

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
µg/L	micrograms per litre
a.i.	active ingredient
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
bw	body weight
CAS No.	Chemical Abstracts Service Number (also referred to as CAS RN)
CFR	Code of Federal Regulations
COC	chemical of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC_{50}	median effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
GLP	Good Laboratory Practice
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilogram per cubic metre
KI	Klimisch scoring system
K_{ow}	n-octanol/water partition coefficient
kPa	kilopascal
LC_{50}	lethal concentration 50%
LD_{50}	lethal dose 50%
LLNA	local lymph node assay
LOAEL	lowest observed adverse effect concentration
LOEC	lowest observed effect concentration
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme

NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	reference dose
SGG	Synthetic Greenhouse Gases
UDS	Unscheduled DNA Synthesis
USEPA	United States Environmental Protection Agency

Attachment 2 Risk Characterisation Tables

Attachment 2, Table 1
Summary of Exposure Point Concentrations

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)[1]	Estimated Concentration in Combined Balance Water Feed Pond to WMF (mg/L)[2]		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[3]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[4]		Estimated Concentration in Dawson River Sediment (mg/kg)[4]	
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)	
					0	30	0	30	0	30	0	30
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	5.40E-02	7.21E-01	7.20E-03	7.20E-04	2.13E-16	7.20E-06	2.13E-18	1.44E-07	4.27E-20	9.01E-08	2.67E-20

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated flowback concentration in pond influent (150% of injected fluid volume) per coal seam per 20% of mass returned calculated using equation: Pond Influent = FBconcentration (mg/L)/ FB dilution 150% x percent mass returned (mg/L)
2) Estimated flowback concentration was multiplied by a factor of 10% to account for dilution in the water feed pond (90:1) due to the aggregation of produced water from other wells which were not recently hydraulically fractured into the same pond.
3) Concentrations in the water feed pond were further reduced by a factor of 99% to account for efficiencies in the WMF system.
4) A dilution factor of 50 was assumed within the approved mixing zone.
5) $EPC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times EPC_{water}$
Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = treated water EPC
$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]
$Kp_{sed} = K_{oc} \times f_{oc}$
Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg), chemical-specific value found in dossier provided in Attachment 1.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

Attachment 2, Table 2
Comparison of Theoretical Concentrations of COPCs to Drinking Water Guidelines

Permeate Pond								
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[1]		Drinking Water Screening Level (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	7.20E-06	2.13E-18	1.44E-07	4.27E-20	6.00E-01	2.4E-07	7.1E-20

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 2, Table 3
Comparison of Theoretical Concentrations of COPCs to PNECs (Water and Sediment)

Permeate Pond														
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[1]		PNEC aquatic (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)		Estimated Concentration in Dawson River Sediment (mg/kg)[1]		PNEC sediment (mg/kg)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30	0	30		0	30
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	7.20E-06	2.13E-18	1.44E-07	4.27E-20	1.40E-04	1.0E-03	3.0E-16	9.01E-08	2.67E-20	5.40E-03	1.7E-05	4.9E-18

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 2, Table 4
Risk Estimates for Cattle Egret - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Avian NOAELt [1]	Avian NOAEL Test Animal		Avian Receptor Cattle Egret	
			Animal	Body Weight (kg)		Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.70E+01	Rat	3.50E-01	2.06E+00	Mallard Duck	1.58E+00	3.90E-01	1.7E+01

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.03	(c)
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	0.39	Siegfried, 1969
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
W.R. Siegfried (1969) Energy Metabolism of the Cattle Egret, ZoologicaAfricana, 4:2, 265-273, DOI: 10.1080/00445096.1969.11447375
c/ Drinking water ingestion rate (WIR) based on the allometric relationship developed by Calder and Braun (1983), where WIR (L/day) = 0.059 x BW $(Kg)^{0.67}$

Constituent Name	CAS No.	EPC [1] Day 0	EPC [1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.4E-07	4.3E-20	1.7E+01	2.1E-10	1.3E-11	6.3E-23	3.8E-24

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 2, Table 5
Risk Estimates for Kangaroo - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Mammal Kangaroo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.70E+01	Rat	3.50E-01	2.50E+01	2.83E-02

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	3	Fleming, 2001
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	25	Fleming, 2001
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
Fleming, 2001
Fleming, Peter; Laurie Corbett, Robert Harden, Peter Thomson (2001). Managing the Impacts of Dingoes and Other Wild Dogs. Commonwealth of Australia: Bureau of Rural Sciences.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.4E-07	4.3E-20	2.8E-02	3.3E-10	1.2E-08	9.8E-23	3.5E-21

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 2, Table 6
Risk Estimates for Dingo - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Dingo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.70E+01	Rat	3.50E-01	1.30E+01	2.83E-02

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weight test}{Body\ Weight receptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.75	Dawson, 1995
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	13	Dawson, 1995
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
Dawson, 1995
Dawson, Terence J. (1995). Kangaroos: Biology of the Largest Marsupials. Cornell University Press, Ithaca, New York. Second printing: 1998. ISBN 0-8014-8262-3.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.4E-07	4.3E-20	2.8E-02	1.6E-10	5.6E-09	4.7E-23	1.7E-21

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 2, Table 7
Risk Estimates for Cattle - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Mammal Cattle	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.70E+01	Rat	3.50E-01	4.54E+02	2.83E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	86	API, 2004
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	454	API, 2004
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
API, 2004
API. (2004). Risk-Based Screening Levels for the Protection of Livestock Exposed to Petroleum Hydrocarbons, Regulatory Analysis and Scientific Affairs No. 4733 July 2004.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9	1.4E-07	4.3E-20	2.8E+00	5.2E-10	1.8E-10	1.5E-22	5.5E-23

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Qualitative and Quantitative Tier 3 Assessment

Cupric Nitrate

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Cupric nitrate is a component in a Water Management Facility (WMF) product used as a biocide during water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1** on the following page.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals – Tier 3 Chemicals

Proprietary Name	Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Biomate MBC781	Cupric Nitrate	3251-23-8	Stabilizer	2 x 1000 L (IBC)*
	Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9		
	Water	7732-18-5		

*estimated volume, product is proposed for use
CAS No = Chemical Abstracts Service Number
IBC = intermediate bulk container
L = litre

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 2**. Since an Australian Drinking Water Guideline (ADWG) Value is available (see **Table 2**), toxicological reference values (TRVs) were not derived for the chemical. A detailed discussion of the drinking water guideline values is presented in **Attachment 2**.

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Cupric Nitrate (3251-23-8)	Copper	2 mg/L (health); 1 mg/L (aesthetics)

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicity reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effect concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are

detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Cupric Nitrate (3251-23-8)	-	-	-	0.0014

$PNEC_{water}$ for cupric nitrate is the ANZG Water Quality Guideline – Freshwater Trigger Value for copper.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Cupric Nitrate (3251-23-8)	-[a]	-	-	87

a – Calculated using weight of evidence approach and an assessment factor of 1.
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Cupric Nitrate (3251-23-8)	-[a]	-	-	65

a -Calculated using a bioavailability regression model and an assessment factor of 1.
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Cupric nitrate is a copper compound. Copper is an inorganic substance and a transition metal with more than one oxidation state. Copper in its metallic form (Cu°) is not available. Copper needs to be transformed to its ionic forms to become available for uptake by living organisms. The principal ionic forms are cuprous (Cu(I), Cu^{+}) and cupric (Cu(II), Cu^{2+}). Among the copper species released/transformed, Cu (II) is thus the most environmentally relevant species. The molecular structure of cupric nitrate is presented in **Figure 1**.

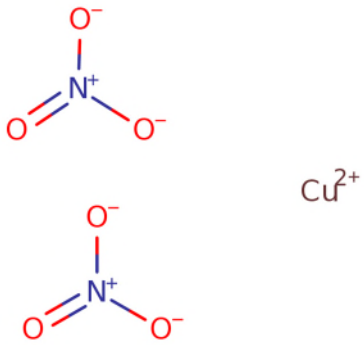

Figure 1 Molecular Structure of Cupric Nitrate[2]

After being released into the environment, Cu(II) ions typically bind to inorganic and organic ligands contained within water, soil, and sediments. In water Cu(II) binds to dissolved organic matter (e. g. humic or fulvic acids). In all environmental compartments (water, sediment, soil), the binding affinities of Cu(II) with inorganic and organic matter is dependent on pH, the oxidation-reduction potential in the local environment, and the presence of competing metal ions and inorganic anions.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for cupric nitrate is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that cupric nitrate is not a PBT substance.

Human Health Hazards

Copper is an essential metal present in human body tissues and fluids at concentrations of parts per million or parts per billion. It is also under tight homeostatic mechanisms that can control excess copper exposure by changing the rate of systemic uptake or excretion via the bile in humans. Therefore, in assessing the human health effects of copper the essentiality and homeostatic mechanisms have to be taken into account.

Cupric nitrate is corrosive to the skin, and it causes serious damage to the eyes. It is not a skin sensitiser. No systemic effects were observed in sub-chronic oral or inhalation toxicity studies. It is not genotoxic, carcinogenic, nor is it a reproductive or developmental toxicant.

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/3251-23-8

TRVs were not derived for cupric nitrate. The health-based ADWG value for copper (2 mg/L) may be applicable (see **Table 2**). A value of 1 mg/L was recommended for aesthetics. Concentrations above 1 mg/L may cause blue or green stains on sanitary ware (ADWG, 2021).

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the treatment process described in **Attachment 1**, cupric nitrate is present as a stabiliser in the WMF product at a *de minimis* concentration of <0.5%. In aqueous solution, cupric nitrate fully dissociates to copper (Cu^{2+}) and nitrate (NO_3^-) anions. During the treatment process, these anions would be removed by the reverse osmosis (RO) system, with the majority directed to brine (i.e., less than 5% to permeate) and subject to immobilization. As a result, this chemical was not evaluated further in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

Copper is an essential micronutrient, needed for optimal growth and development of micro-organisms, plants and animals. Copper and copper compounds may present a hazard for the environment depending on the release/bioaccessibility of copper ions and on the conditions of the receiving environment (pH, hardness, presence and type of organic matter, anions and competing cations).

Cupric nitrate in acute aquatic toxicity studies is very toxic and in chronic aquatic toxicity studies is very toxic with long lasting effects.

PNECs for cupric nitrate are provided in **Tables 3 – 5**. ANZG derived a freshwater high reliability trigger value for copper of 1.4 µg/L using the statistical distribution method at 95% protection (ANZG, 2021). The 95% species protection level for copper in freshwater (1.4 µg/L) is recommended for adoption in the assessment of slightly-to-moderately disturbed ecosystems. Considering the land uses in the vicinity of the WMF, which includes light to moderate grazing, adoption of this level of protection is considered appropriate and was used as the PNEC for water.

The freshwater sediment effect records include 62 high quality single-species chronic sediment toxicity values from 6 different sediment- dwelling species of relevance. The individual NOEC values range between 18.3 mg/kg dry weight and >3,158 mg/kg (min-max value). Large intra-species

variability are observed due to variations in organic carbon (OC) content and acid volatile sulphide (AVS) content of the sediments. A PNEC for sediment (87 mg/kg) was derived for cupric nitrate using a weight of evidence approach and an assessment factor of 1.

The copper terrestrial effects database contains more than 250 high quality, chronic terrestrial toxicity values. The chronic NOECs/EC_{10}s vary between 8.4 mg/kg and 2,402 mg/kg. Considering the importance of bioavailability for reducing the intra-species variability, the database also includes supportive information related to the development/validation of the terrestrial copper bioavailability regression models. The bioavailability regression models are used for normalizing the NOECs. A PNEC for soil (65 mg/kg) was derived for cupric nitrate using the bioavailability regression model and an assessment factor of 1.

PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 2**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

1. Aquatic ecological receptors within Dawson River downstream of the release point
2. Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to cupric nitrate that may occur during water treatment activities. The risk characterisation evaluates the toxicity of this chemical and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, cupric nitrate would not be present in permeate or brine. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), cupric nitrate does not meet the criteria for persistence or bioaccumulation. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 6** below provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 6 Evaluation of Uncertainty – Cupric Nitrate

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentration of cupric nitrate in permeate, brine or treated water was not estimated. The substance, which is present in de minimis concentrations, fully dissociates and no residuals are present. However, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Toxicity Assessment	The use of a weight of evidence approach to derive a PNEC for sediment and the use of a bioavailability regression model to derive a PNEC for soil.	Low to Medium	Low to medium potential to underestimate or overestimate risk

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Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Biomate MBC781	Cupric Nitrate Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT) Water	3251-23-8 55965-84-9 7732-18-5	<0.5 5-12 >85	Biomate MBC781	Suez Water Technologies and Solutions Pty Ltd	Reverse Osmosis Plant	1000L IBC		2 x 1000L (IBC)		TBD		TBD	biocide

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration	
				(mg/L)	Permeate notes	(mg/kg)	mg/kg	(mg/L)	Brine Notes
Biomate MBC781	Cupric Nitrate	3251-23-8	No residual	NA	Cupric nitrate fully dissociates to copper (Cu^{2+}) and nitrate (NO_3^-) anions. These anions are removed by the RO system, (95%) goes to brine, 5% stays within permeate. Residual concentrations are de minimis and subject to immobilization in the pond.	NA	NA	NA	Cupric nitrate fully dissociates to copper (Cu^{2+}) and nitrate (NO_3^-) anions. These anions are removed by the RO system, (95%) goes to brine, 5% stays within permeate. Residual concentrations are de minimis and subject to immobilization in the pond.
	Mixture of 5-chloro-2-methyl-2h-isothiazolol-3-one (CMIT) and 2-methyl-2h-isothiazol-3-one (MIT)	55965-84-9		NA		NA	NA	NA	
	Water	7732-18-5		NA		NA	NA	NA	

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

CUPRIC NITRATE

This dossier on cupric nitrate presents the most critical studies pertinent to the risk assessment of cupric nitrate in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion –Cupric nitrate was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Cupric Nitrate was assessed as a tier 3 chemical for acute and chronic toxicity. Therefore, this substance is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Cupric nitrate is a copper compound. Copper is an inorganic substance and a transition metal with more than one oxidation state. Copper in its metallic form (Cu°) is not available. Copper needs to be transformed to its ionic forms to become available for uptake by living organisms. The principal ionic forms are cuprous (Cu(I), Cu^{+}) and cupric (Cu(II), Cu^{2+}). Among the copper species released/transformed, Cu (II) is thus the most environmentally relevant species.

In humans, copper is an essential metal present in human body tissues and fluids at concentrations of parts per million or parts per billion. It is also under tight homeostatic mechanisms that can control excess copper exposure by changing the rate of systemic uptake or excretion via the bile in humans. Therefore, in assessing the human health effects of copper the essentiality and homeostatic mechanisms have to be taken into account. Cupric nitrate is corrosive to the skin and it causes serious damage to the eyes. It is not a skin sensitiser. No systemic effects were observed in sub-chronic oral or inhalation toxicity studies. It is not genotoxic, carcinogenic, nor is it a reproductive or developmental toxicant.

Likewise in the environment, copper is an essential micronutrient, needed for optimal growth and development of micro-organisms, plants and animals. However, copper and copper compounds may present a hazard for the environment depending on the release/bioaccessibility of copper ions and on the conditions of the receiving environment (pH, hardness, presence and type of organic matter, anions and competing cations). Cupric nitrate in acute aquatic toxicity studies is very toxic and in chronic aquatic toxicity studies is very toxic with long lasting effects.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): copper dinitrate

CAS RN: 3251-23-8

Molecular formula: CuN_2O_6

Molecular weight: 187.56 g/mol

Synonyms: Cupric nitrate; claycop; copper (2+) dinitrate; nitric acid, copper(2+) salt (2:1); copper(II)nitrate

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1: Overview of the Physico-chemical Properties of Cupric Nitrate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Blue crystalline solid	2	ECHA
Melting Point	255°C pressure not indicated	2	ECHA
Boiling Point	266°C @ 101.3 kPa	2	ECHA
Density	2.39 (relative density) @ 20 °C	2	ECHA
Vapor Pressure	0 Pa @ 25°C (estimated value)	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	1450 g/L @ 25°C	2	ECHA
Dissociation constant (pKa)	Not applicable	-	-

Copper is an inorganic substance and a transition metal with more than one oxidation state. The principal ionic forms are cuprous (Cu(I), Cu^{+}) and cupric (Cu(II), Cu^{2+}). Cu^{+} is unstable in aqueous media and soluble Cu^{1+} compounds readily transforms into soluble Cu^{2+} ions, compounds and/or insoluble Cu^{2+} ions, compounds (e.g., copper sulphides) that precipitate. This transformation of Cu^{+} to Cu^{2+} is a result of a redox reaction initiated through atmospheric water vapour as well as in aqueous solution. However, monovalent copper cations are only susceptible to such transformation when they are not chemically bound in insoluble compounds or stabilised in complexed forms. Among the copper species released/transformed, Cu (II) is thus the most environmental relevant species (ECHA).

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for cupric nitrate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No

Convention, Protocol or other international control	Listed Yes or No?
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Copper is a natural element and transition metal with more than one oxidation state. Copper in its metallic form (Cu°) is not available. Copper needs to be transformed to its ionic forms to become available for uptake by living organisms (ECHA).

B. Biodegradation

Biodegradation as used for organic substances does not apply to inorganic substances such as copper and its compounds.

C. Environmental Distribution

After being released into the environment, Cu(II) ions typically bind to inorganic and organic ligands contained within water, soil, and sediments. In water Cu(II) binds to dissolved organic matter (e. g. humic or fulvic acids). The Cu(II) ion forms stable complexes with -NH_2, -SH, and, to a lesser extent, -OH groups in these organic acids. Cu(II) will also bind with varying affinities to inorganic and organic components in sediments and soils. For example, Cu(II) binds strongly to hydrous manganese and iron oxides in clay and to humic acids, but much less strongly to aluminosilicates in sand. In all environmental compartments (water, sediment, soil), the binding affinities of Cu(II) with inorganic and organic matter is dependent on pH, the oxidation-reduction potential in the local environment, and the presence of competing metal ions and inorganic anions (ECHA).

In soil, Cu (II) has a reported soil partition coefficient (Kd) value of 2,120 L/kg (ECHA). Based on this value, if released to soil, the substance is expected to strongly adsorb. As described above, soil pH is a key factor governing attenuation (ECHA).

If released to water, copper binds to the sediment organic carbon (particulate and dissolved) and to the anaerobic sulphides, resulting in the formation of copper sulfide (CuS). CuS has a very low stability constants/solubility limit (LogK=-41, ECHA) and therefore the ‘insoluble’ CuS keeps copper in the anaerobic sediment layers, limiting the potential for remobilization of Cu-ions into the water column (ECHA).

D. Bioaccumulation

Because copper is an essential nutrient, all living organisms have well developed mechanisms for regulating copper intake, copper elimination and internal copper binding. There is a considerable amount of copper accumulation data available, that could potentially be used to calculate bioconcentration factors (BCF) and bioaccumulation factors (BAF) and assess the corresponding

potential risks in aquatic food chains. The information in the accumulation section demonstrates that copper is well regulated in all living organisms and that highest BCF/BAF values are noted when copper concentrations in water, sediments and soils are low and for organisms/ life stages with high nutritional needs. The BCF/BAF values therefore have no ecotoxicological meaning. Importantly, the literature review demonstrates that copper is not biomagnified in aquatic or terrestrial ecosystems (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Copper is an essential metal present in human body tissues and fluids at concentrations of parts per million or parts per billion. It is also under tight homeostatic mechanisms that can control excess copper exposure by changing the rate of systemic uptake or excretion via the bile in humans. Therefore, in assessing the human health effects of copper the essentiality and homeostatic mechanisms have to be taken into account (ECHA).

Cupric nitrate is corrosive to the skin and it causes serious damage to the eyes. It is not a skin sensitiser. No systemic effects were observed in sub-chronic oral or inhalation toxicity studies. It is not genotoxic, carcinogenic, nor is it a reproductive or developmental toxicant.

B. Acute Toxicity

No data available given the fact that this substance is corrosive (ECHA).

C. Irritation

Skin

In an OECD 431 (In vitro skin corrosion: human skin model test) study this substance was determined to be corrosive to the skin (ECHA) [KI. Score =1].

Eyes

Given the fact that this substance is corrosive to the skin it has been assumed to also cause serious eye damage (ECHA).

D. Sensitisation

In an OECD Guideline 406 (Skin Sensitization) study cupric nitrate was determined to be not sensitising to the skin of guinea pigs (ECHA) [KI. Score =1].

E. Repeated Dose Toxicity

Oral

In order to minimise animal testing, studies were conducted using copper (II) sulfate (also referred to as copper sulphate pentahydrate [CAS No. 7758-98-7]). Extensive studies have shown that copper

and copper compounds are considered equally or less bioavailable to a number of animal species when compared to copper sulphate pentahydrate (ECHA).

An EU Method B.26 (Sub-Chronic Oral Toxicity Test: Repeated Dose 90-Day Oral Toxicity Study in Rodents) was performed using male and female F344/N rats. Copper (II) sulfate was administered orally via feed for 92 days at a dose of 0, 500, 1000, 2000, 4000 or 8000 ppm (providing estimated intakes of 0, 8, 17, 34, 67 or 138 mg Cu/kg bw/day). A NOAEL of 1,000 ppm (equivalent to 16.7 mg Cu/kg bw/day was established based on the absence of hyperplasia and hyperkeratosis of the forestomach and absence of inflammation of the liver (ECHA) [KI score = 1].

In a EU Method B. 26 (Subchronic Oral Toxicity Test: Repeated Dose 90-Day Oral Toxicity Study in Rodents) test, male and female B6C3F1 mice were exposed to 0, 1000, 2000, 4000, 8000 or 16000 ppm copper sulphate pentahydrate in their feed for 92 days (providing estimated intakes of 0, 44, 97, 187, 398 and 815 mg Cu/kg bw/day in males and 0, 52, 126, 267, 536 and 1058 mg Cu/kg bw/day in females). The NOAEL for this study was determined to 1000 ppm (44 mg Cu/kg bw/day in males and 52 mg Cu/kg bw/day in females) based on the absence of hyperplasia and hyperkeratosis of the forestomach (ECHA) [KI. Score= 1].

Inhalation

In an OECD Guideline 412 (Subacute Inhalation Toxicity: 28-day study), male and female Sprague-Dawley rats were exposed to cuprous oxide at concentrations of 0.2, 0.4, 0.8 and 2.0 mg/m^3 via whole body inhalation for 28 days, with the addition of a 13 -week recovery period and an evaluation of adaptation to test substance exposure (three intermediate time-points at week 0, week 1, and week 2). Further additional study endpoints were measurements of copper levels in lung tissue, lung lavage fluid, liver, brain, as well as wet/dry lung weight ratio and clinical chemistry and cytology of bronchoalveolar lavage fluid of all animals. The additional study endpoints were designed to aid in the interpretation of any test substance effects. The NOAEL for this study was determined to be ≥ 2 mg/m^3, which is the highest dose tested, based on the lack of findings in the lung weight ratio (ECHA) [KI. Score =1].

F. Genotoxicity

Under normal physiological conditions the availability of free copper is low and most of it would be bound to ceruplasmin and albumin. Therefore, the biological relevance of in vitro tests are unrealistic given the high concentration of free copper in the cell culture growth medium. For this reason, the genotoxicity studies provided below are from *in vivo* studies only (ECHA).

An EU Method B. 12 (Mutagenicity-In Vivo Mammalian Erythrocyte Micronucleus Test) study was performed using CD-1 mice exposed to copper (II) sulfate via oral gavage. Copper (II) sulfate did not induce micronuclei in the polychromatic erythrocytes of the bone marrow of CD-1 mice, which indicates that this substance is not genotoxic (ECHA) [KI score = 1].

An OECD Guideline 486 (Unscheduled DNA Synthesis [UDS] Test with Mammalian Liver Cells *in vivo*) was performed using Wister rats exposed to copper (II) sulfate via oral gavage. The results indicate that copper (II) sulfate is not genotoxic because it did not induce cell repair greater than 1.0% (ECHA) [KI score = 1].

G. Carcinogenicity

Available studies on the carcinogenicity of copper are of limited value to ascertain the carcinogenic potential copper compounds. This is due to the fact that these studies are limited due to shorter exposure periods (<2 years) small sample sizes and limited histopathologic examination. However, when the 3 available studies are assessed on an overall balanced approach, they give useful information as to the carcinogenic potential of copper compounds (ECHA).

These results indicate that copper sulphate and other copper salts do not appear to have carcinogenic potential even at very high dose levels of up to 120 mg Cu/kg/bw/day (ECHA) [Kl. Score =3]. In addition, one of the studies indicates that excess copper may have a protective effect on known carcinogens. In summary, the findings of these studies do not raise concerns with respect to carcinogenic activity (ECHA).

H. Reproductive and Developmental Toxicity

In an EPA OPPTS 870.3800 (Reproduction and Fertility Effects) and OCED Guideline 416 (two-generation reproduction toxicity study) test, Crl:CD rats (30 male and 30 female) were fed diets containing 0, 100, 500, 1000 or 1500 ppm copper sulphate pentahydrate for 70 days. Potentially adverse effects considered to be related to copper sulfate treatment were limited to the 1500 ppm groups and were comprised of decreased spleen weight in P1 adult females, and F1 and F2 male and female weanlings. The maternal toxicity and reproductive toxicity NOAEL was determined to be 1000 ppm, the highest dose at which toxicologically important effects attributable to the test substance were not detected. The dietary concentration of 1000 ppm was equivalent to 19.1, 17.0 and 33.8 mg Cu/kg bw/day for P1 females during premating, gestation and the first 2 weeks of lactation, respectively (ECHA). [Kl. Score = 1].

In an OECD Guideline 414 (Prenatal Developmental Toxicity Study) test, copper hydroxide (CAS No. 1344-69-0) was administered at concentrations of 0, 6, 9, or 18 mg Cu/kg bw to pregnant New Zealand white rabbits by gavage from day 7 to day 28 of gestation. The maternal and foetal NOAEL was 6 mg/kg bw/day, based on maternal weight loss, inappetence, and an increased incidence of a common skeletal variant in foetuses at 9 mg/kg bw/day. Effects on the fetus were considered to be secondary to maternal toxicity and consequently not a specific effect of copper on reproduction. Likewise, maternal effects are considered to be local effects on the stomach in rabbits which result from gavage administration of the substance (ECHA). [Kl. Score = 1].

In a non-guideline study, New Zealand white rabbits were exposed to copper (II) sulfate via oral gavage (0, 7.5, 15 or 30 mg Cu/kg bw/day as copper hydroxide) during Day 7 to Day 28 of gestation. Maternal toxic effects were observed at all dose levels, and they were considered treatment related. Therefore, the maternal NOAEL was determined to be 7.5 mg/kg bw/day based on based on mortality, gastric ulcers, hemolytic anemia, renal damage, increased malformation, reduced foetal weights and increased resorptions. There was evidence of compound-related developmental toxicity at 30 mg Cu/kg bw/day. Mean foetal weights were reduced by 12 % relative to the control group. Foetal resorptions appeared slightly increased at this level and 4 foetuses (2 each from 2 litters) were observed with omphalocele (protrusion of intestines at the umbilicus). No evidence of developmental toxicity was observed at the other dose levels. One foetus of the 7.5 mg Cu/kg bw/day group had anasarca, domed head and a short tail. This finding was considered to be incidental since only one foetus showed these changes and no dose-response was observed.

Therefore, a NOAEL of 15 mg/kg bw/day was established for developmental toxicity (ECHA). [Kl. Score = 2].

I. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for cupric nitrate follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2021).

Non-Cancer

An oral toxicological reference value was not derived for cupric nitrate.

The Australian drinking water guideline values for copper is 2 mg/L. This value is based on the provisional maximum tolerable daily intake value established by the World Health Organization (0.5 mg/kg bw/day) and appears to be a safe level for infants and is just below a level where minor symptoms were observed in adults. A value of 1 mg/L was recommended for aesthetics. Concentrations above 1 mg/L may cause blue or green stains on sanitary ware (ADWG, 2021).

Cancer

Cupric nitrate is not considered a carcinogen. Thus, a cancer reference value was not derived.

J. Human Health Hazard Assessment of Physico-Chemical Properties

Cupric nitrate does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability

However, it does exhibit oxidizing properties (ECHA). [Kl. Score = 1].

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Copper is an essential micronutrient, needed for optimal growth and development of micro-organisms, plants and animals. Copper and copper compounds may present a hazard for the environment depending on the release/bioaccessibility of copper ions and on the conditions of the receiving environment (pH, hardness, presence and type of organic matter, anions and competing cations).

Cupric nitrate in acute aquatic toxicity studies is very toxic and in chronic aquatic toxicity studies is very toxic with long lasting effects.

B. Aquatic Toxicity

Bioavailability of the Cu^{2+} ions in both laboratory tests and in the environment may be affected by abiotic factors, (such as pH, alkalinity, hardness and DOC for the water compartment) and therefore copper bioavailability is considered for the interpretation of the copper effects data. Acute and

chronic aquatic toxicity data compiled by ANZG (ANZG, 2021) is provided within this section and is consistent with the data reported in ECHA.

Acute Studies

USEPA (1985) reported acute toxicity data for copper in freshwater species in 41 genera. At a hardness of 50 mg/L, the values ranged from 17 µg/L for *Ptychocheilus* to 10,000 µg/L for *Acroneuria*. Skidmore & Firth (1983) found the acute toxicity of copper for ten Australian species ranged from 200 µg/L to 7800 µg/L. Bacher & O'Brien (1990) reported a range for Australian species ranged from 40 µg/L to 21,000 µg/L (ANZG, 2021).

Chronic Studies

The ANZG water quality guideline (2021) derived a very high reliability default guideline value (DGVs) for copper in freshwater from 130 data points covering 4 taxonomic groups, and these were adjusted to a common hardness of 30 mg/L as $CaCO_3$, as follows (data are reported as geometric means of NOEC after adjustment from other chronic end-points (pH range was 6.96 to 8.61):

- Fish: 10 species, 2.6 µg/L (*Ptylocheilus oregonensis*, from 7-day LC_{50}) to 131 µg/L (*Pimephales promelas*, 7-day LC_{50}); seven species had geometric means <25 µg/L
- Crustaceans: five species, 1.7 µg/L (*D. pulex* and *G. pulex*, NOEC, reproduction & mortality) to 12.1 µg/L (*Hyalella azteca*, from 10 to 14-day LC_{50})
- Insects: three species, 2.2 µg/L (*Tanytarsus dissimilis*, from 10-day LC*50*) to 11 µg/L (*Chironomus tentans*, 10 to 20-day LC_{50})
- Molluscs: three species, 1.64 µg/L (*Flumicola virens*, from 14-day LC_{50}) to 56.2 µg/L (*Corbicula manilensis*, from 7 to 42-day LC_{50}). The latter figure was not included in calculations as it was outside the pH range.

Additional chronic aquatic toxicity data is found in the ANZG Technical Brief (ANZG, 2021).

C. Sediment Toxicity

The freshwater sediment effect records include 62 high quality single-species chronic NOEC/L(E)C_{10} values from 6 different sediment- dwelling species of relevance. The individual NOEC values range between 18.3 mg/kg dry weight and >3,158 mg/kg (min-max value). Large intra-species variability are observed due to variations in organic carbon (OC) content and acid volatile sulphide (AVS) content of the sediments. Normalization of the effects data for AVS was not possible and therefore only NOEC/(L(E)C_{10} values generated under conditions that represent "aerobic" conditions (Low AVS) were retained (ECHA).

D. Terrestrial Toxicity

The copper terrestrial effects database contains more than 250 high quality, chronic NOEC/EC_{10} values. The chronic NOECs/EC_{10}s vary between 8.4 mg/kg for *Eisenia andrei* (cocoon production) and 2,402 mg/kg (maize respiration). The lowest value is actually below the limit for essentiality for the species (OECD, 2018). As described in ECHA, considering the importance of bioavailability for reducing the intra-species variability, the database includes supportive information related to the development/validation of the terrestrial copper bioavailability regression models. The bioavailability regression models are used for normalizing the NOECs (ECHA).

E. Calculation of PNEC

The PNEC calculations for cupric nitrate follow the methodology discussed in DEWHA (2009).

PNEC water

The ANZG water quality guideline (2021) derived a very high reliability DGV for copper in freshwater. The DGVs for 99, 95, 90 and 80% species protection are 1 µg/L, 1.4 µg/L, 1.8 µg/L and 2.5 µg/L, respectively. The 95% species protection level for copper in freshwater (1.4 µg/L) is recommended for adoption in the assessment of slightly-to-moderately disturbed ecosystems. It applies to waters of hardness of 30 mg/L as $CaCO_3$ (ANZG, 2021).

PNEC sediment

In the ECHA REACH database (ECHA), a $PNEC_{sediment}$ was derived for cupric nitrate using a weight of evidence approach and an assessment factor of 1. The $PNEC_{sediment}$ was determined to be 87 mg/kg sediment dry weight.

PNEC soil

In the ECHA REACH database (ECHA), a $PNEC_{soil}$ was derived for cupric nitrate using a bioavailability regression model and an assessment factor of 1. The $PNEC_{soil}$ was determined to be 65 mg/kg soil dry weight.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REAC Criteria methodology (DEWHA, 2009; ECHA, 2008). Note that PBT assessments are not relevant for metals (ECHA). Despite this, efforts were made to consider PBT for cupric nitrate.

Cupric nitrate is an inorganic substance. Biodegradation is not applicable. For the purposes of this PBT assessment, the persistent criteria are not considered applicable.

Because copper is an essential nutrient, all living organisms have well developed mechanisms for regulating copper intake, copper elimination and internal copper binding. Bioaccumulation is not relevant. Further, copper is not biomagnified in aquatic or terrestrial ecosystems. As a result, bioaccumulation criteria are not considered applicable.

The chronic toxicity data on copper has a NOEC < 0.1 mg/L. Acute E(L)C50 values are < 1 mg/L. Thus, cupric nitrate does meet the criteria for toxicity.

The overall conclusion is that cupric nitrate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for cupric nitrate.

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9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Cupric nitrate	3251-23-8	Not a PBT	No	No	NA	No	NA	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative risk assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
HHRA	enHealth Human Risk Assessment
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
KI	Klimisch scoring system
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrammes per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
ppb	parts per billion
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency

Qualitative and Quantitative Tier 3 Assessment

Glutaraldehyde

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Glutaraldehyde is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to improve formation permeability, enhancing the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Glutaraldehyde	111-30-8	Antimicrobial	0.000008%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

Glutaraldehyde is also a component in a water treatment product used to provide corrosion resistance from microbial influenced corrosion in the steel flowlines and spinelines in the produced water management collection system. Process and usage information for this chemical is summarised in **Table 2**.

Table 2 Water Management Facility Chemicals

Chemical Name	CAS No.	Use	Percent Weight (%) in Product[1]
Glutaraldehyde	111-30-8	Antimicrobial	20

[1] Mid-point of range provided in SDS.
CAS No = Chemical Abstracts Service Number

The water treatment product containing glutaraldehyde could potentially be used for biocide treatment in FAPA but is currently not being used. Based on its use in other Santos project areas, dosage rates in water for this chemical in the biocide are in the range of 4.2×10^{-4} mg/L (refer **Attachment 1**). Based on the estimated low concentration in amended blended produced water (2.9×10^{-9} mg/L) resulting from water treatment, this assessment focuses on glutaraldehyde in hydraulic fracturing fluids.

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Glutaraldehyde is not a carcinogen, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 3** provides a summary of the derivation.

Table 3 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Glutaraldehyde (111-30-8)	2-year rat drinking water	Reduced body wt., body wt. gain, food consumption	4	100	0.04	0.14

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
wt = weight
Refer to **Attachment 2** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 4 presents the chemical, endpoint, no observed effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 5** and **6**, respectively. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 4 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Glutaraldehyde (111-30-2)	Chronic algae	0.025	10	0.0025

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 5 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Glutaraldehyde (111-30-2)	[a]	-	-	0.006

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 6 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Glutaraldehyde (111-30-2)	Chronic soil organisms	1.12	50	0.02

EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Glutaraldehyde is a liquid at room temperature. When in the environment, glutaraldehyde is generally in the aquatic phase. The molecular structure of glutaraldehyde is presented in **Figure 1**.

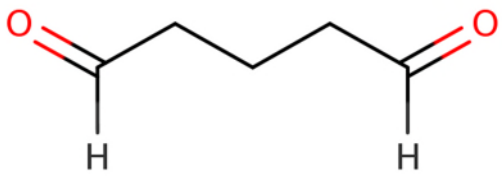

Figure 1 Molecular Structure of Glutaraldehyde[2]

Glutaraldehyde is considered readily biodegradable. It is also expected to have a low potential for bioaccumulation. The organic carbon/water partition coefficients (K_{oc}) values for glutaraldehyde indicate that it will have low potential for adsorption to suspended solids and sediment in water and moderate adsorption to soil. Glutaraldehyde is not expected to undergo hydrolysis in the environment. Overall, glutaraldehyde shows limited persistence in the environment.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for glutaraldehyde is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that glutaraldehyde is not a PBT substance.

Human Health Hazards

Glutaraldehyde has moderate-to-high acute toxicity by the oral route, low-to-moderate toxicity by the dermal route and moderate-to-high toxicity by the inhalation route. Acute inhalation exposure

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/111-30-8

may cause respiratory irritation. Glutaraldehyde is corrosive to the skin and eyes; it is also a skin and respiratory sensitiser.

Repeated oral exposures via drinking water to rats have resulted in general systemic toxicity, but no target organ effects. In contrast, the upper respiratory tract, particularly the nasal cavity, is the target organ in rodents from repeated inhalation exposure. Glutaraldehyde may exhibit weak genotoxic effects in some *in vitro* tests, whereas the *in vivo* studies consistently show no genotoxic activity. Glutaraldehyde is not a reproductive toxicant; developmental toxicity can occur at maternally toxic doses, but there is no teratogenicity. Glutaraldehyde is not a carcinogen.

Based on a review of repeated dose and developmental toxicity studies, toxicological reference values were derived for glutaraldehyde. The drinking water guideline value derived for glutaraldehyde using the non-carcinogenic oral RfD is 0.14 mg/L.

Glutaraldehyde may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

There is low potential for human receptors to be exposed to glutaraldehyde in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, glutaraldehyde is considered readily biodegradable in an aerobic aquatic environment with a half-life of 10.6 hours in the water/sediment system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an ‘Unnamed tributary of the Dawson River’, not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

Glutaraldehyde has a moderate acute toxicity concern to fish and invertebrates but is highly toxic to algae. It is of low toxicity concern to terrestrial invertebrates and plants. To birds, glutaraldehyde is moderately toxic on an acute basis and slightly toxic on a subacute dietary basis. Under typical environmental conditions, the chemical is readily biodegradable and has limited persistence in the environment. The chemical also has a low potential for bioaccumulation.

Experimental toxicity data on water and soil organisms was available for three trophic levels to calculate PNECs. However, there are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released produced water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to glutaraldehyde that may occur during hydraulic fracturing and work over activities. The risk characterisation evaluates the toxicity of this chemical and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio

of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Exposure Point Concentration. Calculations

A quantitative mass balance calculation was undertaken to estimate the potential concentrations of stimulation chemicals containing glutaraldehyde within diluted produced water. For the mass balance calculation, vendor disclosure forms were used to determine the percentage of glutaraldehyde in the pre-injection fluid. **Table 7** presents the estimated pre-injection fluid concentration.

Table 7 Mass Balance Estimates for Glutaraldehyde

Chemical Name	CAS No.	Estimated Pre-injection fluid concentration (mg/L)
Glutaraldehyde	111-30-8	0.0008

CAS No = Chemical Abstracts Service Number
mg/kg = milligram per kilogram
mg/L = milligram per litre

The mass balance of glutaraldehyde was then used to estimate potential EPCs for the evaluation of treated water to the Dawson River. The potential EPCs have been conservatively estimated.

First, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to the surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The biodegradation information was obtained from the OECD ready tests (OECD, 1992) that were developed as a first-tier testing scheme to provide preliminary screening of organic chemicals. The ready tests are stringent screening tests that are conducted under aerobic conditions in which a high concentration of the test substance is used, and biodegradation is measured by non-specific parameters including dissolved organic carbon, biochemical oxygen demand and carbon dioxide production. **Attachment 3, Table 1** includes the environmental fate information that was used to assess biodegradation of the chemical.

The concentrations in the water feed pond were then further reduced by a factor of 99% to account for efficiencies in the WMF system.

Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*.

This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

These estimated surface water EPCs were used to derive EPCs for sediment using the equilibrium partitioning method. **Attachment 3, Table 1** includes the equation and environmental fate information used to derive the sediment EPC.

Release Scenario Assessment

There is no potentially complete exposure pathway to sources of drinking water; however, as a conservative measure, the theoretical concentrations for the release scenarios were compared to human health toxicity-based screening levels to screen for potential effects as a result of a release to surface water used as a drinking water source. The results of this comparison, including the ratio of exceedance of screening levels, is presented in **Attachment 3, Table 2**. As detailed in the table, the risk ratio did not exceed the target level of 1 for any of the scenarios.

Theoretical concentrations were also compared to the PNEC for aquatic receptors. **Attachment 3, Table 3** presents the results of this comparison, including the ratio of exceedance of screening levels. Similar to above, risk ratios did not exceed the target level of 1.

The primary land use within the development area is agricultural (grazing on improved or unimproved pastures), and it is sparsely populated. To further evaluate potential risks to non-MNES receptors (mammals and avian), additional quantitative analysis of the managed releases to Dawson River was conducted.

Terrestrial receptors evaluated for exposure to Dawson River discharge include domesticated livestock, large mammalian wildlife and small mammalian wildlife. Beef cattle were used to evaluate domesticated livestock, kangaroos were evaluated for large mammalian wildlife, and dingos were evaluated for small mammalian wildlife. The cattle egret was selected to evaluate avian exposures. Exposure assumptions, TRVs and total intake calculations are detailed in **Attachment 3, Tables 4, 5, 6 and 7**. **Attachment 3, Table 4** presents the calculated risk estimates for the kangaroo. **Attachment 3, Table 5** presents the calculated risk estimates for the dingo. **Attachment 3, Table 6** presents the calculated risk estimates for the cattle. **Attachment 3, Table 7** presents the calculated risk estimates for the cattle egret. As indicated in the tables, the calculated HQ for glutaraldehyde did not exceed the risk threshold level of 1 for any of the scenarios evaluated.

Cumulative Impacts

The potential for cumulative impacts associated with chemicals used during stimulation activities is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), glutaraldehyde does not meet the criteria for persistence or bioaccumulation. Further, estimated concentrations in surface water and sediment were less than

PNECs. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 8** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 8 Evaluation of Uncertainty – Glutaraldehyde

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in residual stimulation fluids were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Exposure Assessment	The use of the food consumption relationship with body weight for mammalian and avian receptors.	Low to Medium	Low to medium potential to underestimate or overestimate risk
Toxicity Assessment	The use of toxicity values in a risk assessment is based on extrapolations from animal data, adjust factors for inherent uncertainty in the toxicological estimate and use of surrogate toxicity criteria	Low	Low potential to underestimate risk
Toxicity Assessment	The use of LOAEL/NOAEL for calculation of the TRVs	Low to Medium	Low to medium potential to underestimate or overestimate risk
Toxicity Assessment	The use of the allometric scaling method to estimate the population-level effects on wildlife based on individual level of exposures.	Low to Medium	Low to medium potential to underestimate or overestimate risk

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Attachment 1 Contingency Biocide Dosing Assumptions

Attachment 1
Summary of Exposure Point Concentration Development
(Contingency Water Treatment Chemicals)

Mass Balance

In other Santos project areas, approximately 413 milligrams per litre (mg/L) of a water treatment product is being dosed (9.2 litres [L] added to approximately 1,380 billion barrels [bbl] or 2.2 x 10^5 litres of legacy/CF1 PFW). The constituent of potential concern (COPC) legacy/CF1 produced formation water (PFW) concentrations are calculated based on the product dose that is apportioned between the COPCs based on the COPC percent weight in the product (composition information in the safety data sheet). The concentration of the COPCs in the water storage pond influent (representative of treatment of combined produced water from legacy/CF1 PFW and bore water) was based on the combined dilution from 2,300 bbl/day.

On this basis, the concentration of COPCs in the water storage pond influent are calculated as follows:

COPC	CAS Number	Percent Weight Product	COPC Legacy/CF1 PFW (mg/L)	Storage Pond Influent (mg/L)
Glutaraldehyde	111-30-8	20	4.2E-04	2.9E-09

CAS = Chemical Abstracts Service
COPC = constituent of potential concern
mg/L = milligrams per litre
PFW = produced formation water

Attachment 2 Risk Assessment Dossier

GLUTARALDEHYDE

This dossier on glutaraldehyde presents the most critical studies pertinent to the risk assessment of glutaraldehyde in its use in drilling muds and hydraulic fracturing fluids. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from NICNAS (1994) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Glutaraldehyde was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Glutaraldehyde was assessed as a tier 3 chemical for acute toxicity and as a tier 2 chemical for chronic toxicity. Therefore, glutaraldehyde is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Glutaraldehyde is a liquid at room temperature. It is readily biodegradable and is expected to have a low potential for bioaccumulation. Glutaraldehyde is moderately to highly toxic by the oral route, low to moderately toxic by the dermal route, and moderately to highly toxic by the inhalation route. Acute inhalation exposure may cause respiratory irritation. Glutaraldehyde is corrosive to the skin and eyes; and it is a skin and respiratory sensitiser. Repeated oral exposures via drinking water to rats have resulted in general systemic toxicity, but no target organ effects. In contract, the upper respiratory tract, particularly the nasal cavity, is the target organ in rats and mice from repeated inhalation exposure. Glutaraldehyde may exhibit weak genotoxic effects in some in vitro tests, whereas the in vivo studies consistently show no genotoxic activity. Glutaraldehyde is not a reproductive toxicant; developmental toxicity can occur at maternally toxic doses, but there is no teratogenicity. Glutaraldehyde is slightly to moderately toxic to fish and invertebrates, and moderately to highly toxic to algae. It is of low toxic concern to terrestrial invertebrates and plants.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Glutaraldehyde

CAS RN: 111-30-8

Molecular formula: C7H8O2

Molecular weight: 100.12

Synonyms: Pentanedial; glutaral; glutaric dialdehyde; 1,3-diformylpropane; 1,5-pentanedial; glutaric aldehyde; glutaric acid dialdehyde; dioxopentane; glutardialdehyde; 1,5-pentanedione; Algicide®C

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-Chemical Properties of Glutaraldehyde

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa*	Sweetish smelling, clear water liquid	1	ECHA
Melting Point*	-33°C	1	ECHA
Boiling Point*	101.5°C @ 987.1 hPa	1	ECHA
Density*	1.13 kg/m^3	1	ECHA
Vapour Pressure*	30 hPa @ 26.3°C	1	ECHA
Partition Coefficient (log K_{ow})*	-0.36	1	ECHA
Water Solubility*	miscible	2	ECHA
Flash Point*	Not measurable	1	ECHA
Auto flammability*	395°C @ ~1,000hPa	1	ECHA
Viscosity*	12.75 mm^2/s (static) at 25°C	1	ECHA
Henry's Law Constant	0.011 Pa m^3/mol at 25°C [QSAR]	2	ECHA

*ca. 50% glutaraldehyde solution (in water)
1 ppm = 4.095 mg/m^3
1 mg/m^3 = 0.244 ppm

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for glutaraldehyde.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Glutaraldehyde is considered readily biodegradable. It is also expected to have a low potential for bioaccumulation. The K_{oc} values for glutaraldehyde indicate that it will have low potential for adsorption to suspended solids and sediment in water and moderate adsorption to soil. Glutaraldehyde is not expected to undergo hydrolysis in the environment. Overall, glutaraldehyde shows limited persistence in the environment.

B. Abiotic Degradation

Hydrolysis

In an OECD TG 111 test (hydrolysis as a function of pH), glutaraldehyde was hydrolytically stable at pH 4 and pH 7, but decomposed at pH 9 (ECHA). [Kl. score = 2]

Phototransformation in Water

Photolytic degradation of glutaraldehyde occurred in water under sensitised conditions: the half-life was 18 days when equivalent to 36 days of natural sunlight (12 hours/day; sensitised acetone system); and 49 days when equivalent to 34 days of natural sunlight (12 hours/day; sensitised acetonitrile system). There was no photodegradation of glutaraldehyde under darkness or non-sensitised conditions (ECHA). [Kl. score = 2]

C. Biodegradation

Glutaraldehyde was considered readily biodegradable in an OECD 301A (DOC die away test). Degradation was 90-100% in 28 days (ECHA). [Kl. score = 1]

In a simulation test involving aerobic sewage treatment [activated sludge units] (OECD TG 303A), glutaraldehyde degraded 97% after 73 days based on DOC removal (ECHA). [Kl. score = 1]

In an aerobic aquatic metabolism test, [^{14}C]-glutaraldehyde had a half-life of 10.6 hours in the water/sediment system. A minor transformation product was glutaric acid: the maximum yield was 18.9 to 21.5% at 12 hours, which then declined rapidly to 10.1 to 11% by 24 hours; and was not observed at the end of the study period in the aqueous phase (ECHA). [Kl. score = 1]

In an anaerobic aquatic metabolism test, [^{14}C]-glutaraldehyde was rapidly metabolised with the first-order half-life being 7.7 hours. Glutaraldehyde was transformed to 5-hydroxypentanal (ca 37% of applied radioactivity) on day 1; after that, it declined to <10%; it was not detected at all after 30 days. The second stable transformation product was 1,5-pentanediol (35% of radioactivity on day 1), which accounted for 70% of the radioactivity at the end of the test. A minor transformation product was a compound formed via Aldol condensation, cyclisation and dehydration. This compound accounted for about 10-20% of total radioactivity from day 1 onwards (ECHA). [Kl. score = 1]

In an aerobic soil metabolism test, the half-life of the degradation of [^{14}C]-glutaraldehyde was calculated to be 1.7 days, indicating rapid degradation in soil by microbial biotransformation. Degradation products were measured but not identified. (ECHA). [Kl. score = 1]

D. Environmental Distribution

Adsorption/desorption

The organic carbon/water partition coefficients (K_{oc}) values were determined for sediment and four types of soil. The values are as follows: 120 for sediment; 210 for sandy loam; 500 for silty clay loam; 340 for silt loam; and 460 for loamy sand (ECHA; Leung, 2001). [Kl. score = 1]

Distribution Modelling

No fugacity calculations were performed as glutaraldehyde has limited persistence. Its environmental fate is primarily determined by degradation rather than equilibration between compartments (OECD, 1995).

E. Bioaccumulation

Glutaraldehyde is not expected to bioaccumulate. The measured log K_{ow} at pH 5, 7 and 9 are -0.41, -0.36 and -0.80, respectively (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Glutaraldehyde has moderate-to-high acute toxicity by the oral route, low-to-moderate toxicity by the dermal route, and moderate-to-high toxicity by the inhalation route. Acute inhalation exposure may cause respiratory irritation. Glutaraldehyde is corrosive to the skin and eyes; it is also a skin and respiratory sensitiser. Repeated oral exposures via drinking water to rats have resulted in general systemic toxicity, but no target organ effects. In contrast, the upper respiratory tract, particularly the nasal cavity, is the target organ in rodents from repeated inhalation exposure. Glutaraldehyde may exhibit weak genotoxic effects in some *in vitro* tests, whereas the *in vivo* studies consistently show no genotoxic activity. Glutaraldehyde is not a reproductive toxicant; developmental toxicity can occur at maternally toxic doses, but there is no teratogenicity.

B. Toxicokinetics

Dermal Absorption

[1,5-^{14}C]-glutaraldehyde was applied to the skin of male and female F344 rats. Doses were 0.75% and 7.5%: this corresponds to approximately 6.5 and 63 mg/kg for males; and approximately 8.7 and 102 mg/kg for females. The dermal absorption data are presented below in Table 3. The results indicate that glutaraldehyde has a low rate of absorption by the dermal route (ECHA).

Table 3 Dermal Absorption Data in Rats on Glutaraldehyde (ECHA)

Sex	Absorption rate constant/hour		% of applied dose	
	Low Dose	High Dose	Low Dose	High Dose
Males	1.5	0.7	0.7	1.3
Females	1.8	0.9	0.3	2.1

An *in vitro* percutaneous absorption study was conducted on glutaraldehyde using excised skin from rats, rabbits, mice, guinea pigs and humans. The skin samples were placed in a flow-through skin penetration chamber, and [^{14}C]-glutaraldehyde was added at doses of 0.75% and 7.5%. The results are presented in Table 4. Glutaraldehyde did not penetrate any of the skin samples to a significant degree, suggesting that only minimal amounts of glutaraldehyde may be available for systemic uptake and distribution after skin exposure. The results also show that skin absorption was greater for the animal species used in toxicity tests than human skin (ECHA; Frantz et al., 1993).

Table 4 *In vitro* Percutaneous Absorption (mg/cm^2) of Glutaraldehyde (ECHA; Frantz et al., 1993)

Species	Low Dose	High Dose
Animal*	0.006	0.08
Human	0.002	0.02

*Percutaneous absorption in rats, guinea pigs, mice and rabbits were similar to each and were reported as a single value.

C. Acute Toxicity

The oral LD_{50} values are: 123 to 820 mg/kg in rats; 100 to 352 mg/kg in mice; and 50 mg/kg in guinea pigs (NICNAS, 1994).

The dermal LD_{50} values are: 640 to 2,000 mg/kg in rabbits; >2,500 mg/kg in rats; and >4,500 mg/kg in mice (NICNAS, 1994).

The 4-hour inhalation LC_{50} values for glutaraldehyde are listed in Table 5.

Table 5 Acute inhalation LC_{50} values for Glutaraldehyde

Test Material	LC_{50} (males) [mg/L]	LC_{50} (females) [mg/L]	LC_{50} (both sexes) [mg/L]	Reference
50% aq. aerosol	0.52	0.45	-	OECD, 1995
25% aq. aerosol	-	-	0.8	OECD, 1995
50% aq. aerosol	0.35	0.28	-	OECD, 1995
5% soln. vapour	0.096	0.164	-	OECD, 1995

During the exposure period, the animals showed signs of eye and respiratory irritation, as indicated by laboured and audible breathing, and wetness and encrustation around the nose and eyes.

D. Irritation

Glutaraldehyde is corrosive to the skin and eyes of rabbits (NICNAS, 1994; ECHA). Signs of irritation occurred at a concentration of 2% for skin and 0.2% for eyes (NICNAS, 1994). In the acute inhalation studies, rats exposed to aerosols or vapours of glutaraldehyde showed signs of eye and respiratory irritation (OECD, 1995).

E. Sensitisation

Glutaraldehyde is a skin sensitiser to guinea pigs and humans. Information on the individual studies can be found in NICNAS (1994) and in the ECHA REACH database (ECHA).

Asthmatic symptoms, such as wheezing, coughing, chest tightness, breathing difficulties and non-specific hyper-responsiveness, have been reported to occur in humans occupationally exposed to glutaraldehyde (NICNAS, 1994). It is unclear whether the asthma is an allergic hypersensitivity response or a result of the aggravation of pre-existing asthma due to the irritating properties of glutaraldehyde. Nevertheless, glutaraldehyde should be considered a respiratory sensitiser, although one of low potency.

F. Repeated Dose Toxicity

Oral

Male and female Wistar rats were given in their drinking water 0, 100, 500 or 2,000 ppm glutaraldehyde for 90 days. The approximate daily intakes were 0, 3, 15 or 53 mg/kg-day for males, and 0, 4, 19 or 72 mg/kg-day for females. There were no signs of neurotoxicity at any dose level. There was slight impairment of food consumption in the 2,000 ppm animals, as well as slight impairment of body weight and body weight gain. Impaired water consumption was seen in the 100 and 500 ppm females. The NOAEL for males is 500 ppm (15 mg/kg-day). The NOAEL for females is 100 ppm (4 mg/kg-day), since the impaired water consumption in the 100 ppm females was considered a palatability problem and not an adverse effect (ECHA). [Kl. score = 1]

Male and female F344 rats were given in their drinking water 0, 50, 250 or 1,000 ppm glutaraldehyde for 13 weeks. Additional groups of animals were given in their drinking water 0 or 1000 ppm glutaraldehyde for 13 weeks followed by a 4-week recovery period. The approximate daily intakes were 0, 5, 25 or 100 mg/kg-day for males; and 0, 7, 35 or 120 mg/kg-day for females. Water consumption was reduced in a dose-dependent manner in the $\geq$250 ppm males and 1,000 ppm females, which was attributed to an aversion to the taste and/or odour of glutaraldehyde in the water. There was also a reduction in food consumption in the 1,000 ppm animals with a parallel reduction in body weights. It is unclear whether the reduction in food consumption was related to the decreased water consumption. Urine volume was decreased with an increase in specific gravity, along with a slight increase in protein and ketone concentration, in the $\geq$250 ppm animals, which was probably related to the decreased water consumption. There were no treatment-related changes in the haematology parameters measured. Blood urea nitrogen was increased in a dose-related manner in the $\geq$250 ppm females at the 6-week time point, but at the 13-week or 17-week time points. Relative kidney weights were increased in a dose-related manner in the $\geq$250 ppm males and females, and increased absolute kidney weights in the females. Histopathological examination showed no treatment-related effects. The NOAEL is 50 ppm (5 and 7 mg/kg-day for

males and females, respectively) based on dose-related increase in kidney weights at ≥250 ppm (ECHA). [Kl. score = 2]

Male and female Wistar rats were given in their drinking water 0, 100, 500 or 2000 ppm glutaraldehyde for 12 months. The approximate daily intakes were: 0, 6.4, 30.5 or 116.6 mg/kg-day for males; and 0. 9.6, 46 or 153 mg/kg-day for females. There was no treatment-related mortality. At 2,000 ppm, treatment-related effects included respiratory sounds (both sexes), decrease in body weight (males), decrease in body weight gain (both sexes), decrease in food consumption (both sexes), reduced water consumption (both sexes), lesions within the glandular stomach (both sexes showed erosion/ulceration of the glandular stomach), increased incidence of clear cell foci in the liver (males) and a single case of slight diffuse squamous metaplasia in the epithelium of the larynx (male). At 500 ppm, water consumption was reduced in males which was considered to be a palatability (bad taste) problem and not an adverse effect. No effects were seen in the 100 ppm animals. The NOAEL for this study is 500 ppm, which corresponds to 30.5 and 46 mg/kg-day for males and females, respectively (ECHA). [Kl. score = 1]

Male and female Fischer 344 rats were given in their drinking water 0, 50, 250 or 1000 ppm glutaraldehyde for 104 weeks. The mean glutaraldehyde consumption was 0, 4, 17 and 64 mg/kg-day for males and 0, 6, 25 and 86 mg/kg-day for females. There were no treatment-related mortalities or clinical symptoms of toxicity. In the 250 and 1,000 ppm groups, there was reduction in body weight and body weight gain; reduction in food and water consumption; increased statistically significant incidence of nucleated erythrocytes and of large monocytes; decreases in alanine aminotransferase (ALT), aspartate aminotransferase (AST), and glutamate dehydrogenase; dose-related decrease in urine volume accompanied by a dose-related increase in osmolality; changes in absolute and relative kidney weight; gastric irritation; increases in bone marrow hyperplasia; and increased incidence of renal tubular pigmentation. The decreased water consumption was considered to be due to the bad taste, smell and/or irritancy of the test substance in the drinking water; thus, it is of no toxicological relevance. As a result of reduced water intake, there are renal physiological adaptation, such as decreased urine, increased osmolality and changes in kidney weight. The haematological and clinical chemistry parameter changes were marginal and were considered to be of no toxicological relevance. The main haematological finding seen at the end of the study and which consisted of the appearance of nucleated erythrocytes and large monocytes in all treated groups (statistically significant for the ≥250 ppm males) was related to the incidence of large granular lymphocytic leukaemia (LGLL) in the spleen. The bone marrow hyperplasia and renal tubular pigmentation are related to the occurrence/incidence of LGLL, and were considered by the authors of the study as being secondary to a low grade haemolytic anaemia in animals with LGLL. The NOAEL for this study is 50 ppm which corresponds to 4 and 6 mg/kg-day for males and females, respectively (Van Miller *et al.* 2002). [Kl. score = 2]

Inhalation

Male and female F344 rats were exposed by inhalation to 0, 0.0625, 0.125, 0.25, 0.5 or 1.0 ppm (0, 0.26, 0.5, 1, 2 or 4.1 mg/m^3) glutaraldehyde for 6.5 hours/day, 5 days/week for 13 weeks. The study focused on the respiratory tract, using histopathology and epithelial cell labelling index as end points. Histopathological lesions in the nasal passages and turbinates were seen at ≥0.25 ppm. Treatment-related effects were primarily the respiratory mucosa (nasal cavity and tips of the turbinates) and the olfactory epithelium (dorsal meatus). Hyperplasia, squamous metaplasia, olfactory degeneration, squamous exfoliation (accumulation of keratin, cell debris and bacteria in

the lumen of the nasal vestibule) and focal erosions were reported for both sexes, and the severity and incidence of the findings increased with increasing concentration of glutaraldehyde. The NOAEL for this study is 0.125 ppm (Gross et al., 1994). [Kl. score = 1]

Male and female B6C3F$_1$ mice were exposed by inhalation to 0, 0.0625, 0.125, 0.25, 0.5 or 1.0 ppm (0, 0.26, 0.5, 1, 2 or 4.1 mg/m^3) glutaraldehyde for 6.5 hours/day, 5 days/week for 13 weeks. The study focused on the respiratory tract, using histopathology and epithelial cell labelling index as end points. Histopathologic lesions in the nasal passages and turbinates were seen at all exposure concentrations ($\geq$0.0625 ppm). Treatment-related lesions were primarily the respiratory mucosa (nasal cavity and tips of the turbinates) and the olfactory epithelium (dorsal meatus). Hyperplasia, squamous metaplasia, olfactory degeneration, squamous exfoliation (accumulation of keratin, cell debris and bacteria in the lumen of the nasal vestibule) and focal erosions were reported for both sexes, and the severity and incidence of the findings increased with increasing test concentration. Furthermore, neutrophilic inflammation was seen at $\geq$0.062 ppm, and squamous metaplasia as well as necrosis were seen in the larynx at 1 ppm). The LOAEL for this study is 0.0625 ppm; a NOAEL was not established (Gross et al., 1994). [Kl. score = 1]

Male and female B6C3F$_1$ mice were exposed by inhalation to 0 or 0.1 ppm (0 or 0.41 mg/m^3) glutaraldehyde for 6 hours/day, 5 days/week for 52 and 78 weeks. Survival was similar between treated and control groups. Hyperplasia of the squamous epithelium lining of the dorsal wall of the nasal passages and the lateral aspect of the atrioturbinate was seen in a greater number of exposed females than in controls. Epidermal erosion and ulceration as well as squamous and inflammatory exfoliation were also seen in the nasal lumens. All of these changes were dependent on the length of glutaraldehyde exposure. The authors concluded that, since the induced lesions occurred in the more anterior part of the nasal passages, that they were likely the result of an irritation mechanism (Zissu et al., 1998). [Kl. score = 2]

Male and female Fischer 344 rats were exposed by inhalation to 0, 0.25, 0.5 or 0.75 ppm (0, 1, 2 or 3.1 mg/m^3) glutaraldehyde for 6 hours/day, 5 days/week for two years. Survival in the mid- and high-dose females was statistically significantly decreased compared to controls. Mean body weights of all exposed males and the mid- and high-dose females were generally less than those of the controls. Non-neoplastic lesions were limited primarily to the most anterior region of the nasal cavity. Effects included hyperplasia and inflammation of the squamous epithelium; hyperplasia, goblet cell hyperplasia, inflammation, and squamous metaplasia of the respiratory epithelium; and hyaline degeneration of the olfactory epithelium. The LOAEL for this study is 0.25 ppm based on hyperplasia and inflammation of the squamous epithelium of the nose in both sexes. A NOAEL was not established (van Birgelen et al., 2000). [Kl. score = 2]

Male and female B6C3F$_1$ mice were exposed by inhalation to 0, 0.0625, 0.125 or 0.25 ppm (0, 0.26, 0.5 or 1 mg/m^3) glutaraldehyde for 6 hours/day, 5 days/week for two years. Survival of the treated animals was similar to controls. Mean body weights of the high-dose females were generally lower than the controls. Non-neoplastic lesions were limited primarily to the anterior region of the nasal cavity; the effects were qualitatively similar to those seen in the rats Squamous metaplasia of the respiratory epithelium was observed in both sexes of mice while female mice also had inflammation and hyaline degeneration of the respiratory epithelium. The incidence and severity grade (in parentheses) of the hyaline degeneration were: 16/50 (1.4), 35/49 (1.4), 32/50 (1.3) and 30/50 (1.1) for the 0, 0.0625, 0.125 and 0.25 ppm dose groups, respectively. The LOAEL for this study is 0.0625

ppm based on hyaline degeneration of the respiratory epithelium in female mice. A NOAEL was not established (van Birgelen et al., 2000). [Kl. score = 2]

Dermal

Applications of a 50% solution of glutaraldehyde was applied to the skin of male and female SD rats for 13 weeks. The doses were 0, 50, 100 and 150 mg/kg glutaraldehyde. At the application site, there were signs of irritation (scabs, desquamation and very slight or well-defined erythema). There was no treatment-related mortality, clinical signs, body weights, feed consumption and ophthalmoscopic effects. There were no changes in the haematology and clinical chemistry parameters that were considered to be biologically or toxicologically relevant. Organ weights were similar between treated and control animals. Histopathological examination showed treatment-related effects in the skin associated with chronic irritation; no other changes were noted that were considered to be treatment-related. The NOAEL for this study is 150 mg/kg, the highest dose tested (ECHA). [Kl. score = 1]

G. Genotoxicity

In Vitro Studies

Glutaraldehyde may exhibit weak genotoxic effects in some *in vitro* tests. The bacterial reverse mutation assays have been the most consistent. Variable results have been reported for the forward gene mutation tests; and for sister chromatid exchange (SCE), chromosomal aberration and Unscheduled DNA Synthesis (UDS) tests (Vergnes and Ballantyne, 2002).

In Vivo Studies

The *in vivo* studies conducted on glutaraldehyde are presented in Table 6. All of the studies show that glutaraldehyde is not mutagenic or genotoxic.

Table 6 *In Vivo* Genotoxicity Studies on Glutaraldehyde

Test System	Results*	Klimisch Score	Reference
Rat bone marrow (chromosomal aberration)	-	1	ECHA
Rat bone marrow (chromosomal aberration)	-	2	ECHA
Mouse bone marrow (micronucleus)	-	1	ECHA
Rat bone marrow (chromosomal aberration)	-	2	ECHA
Rat germ cell cytogenetic assay (alkaline elution)	-	2	ECHA
Drosophila SLRL Test	-	2	ECHA
Rat liver UDS Assay	-	1	ECHA
Rat germ cell cytogenetic assay (alkaline elution)	-	2	ECHA
Mouse peripheral blood micronucleus study	-	2	Vergnes and Ballantyne (2002)
Rat liver UDS Assay	-	2	Mirsalis *et al.* (1989)

a+, positive; -, negative

H. Carcinogenicity

Oral

Male and female Fischer 344 rats were given in their drinking water 0, 50, 250 or 1,000 ppm glutaraldehyde for 104 weeks. The mean glutaraldehyde consumption was 0, 4, 17 and 64 mg/kg-day for males and 0, 6, 25 and 86 mg/kg-day for females. Mortality rates were 25-30% and 19-23% for males and females, respectively, with no dose-related increase. The major cause of death in all dose groups including the controls was LGLL. There was an increased incidence of LGLL in the liver and spleen in all treated females (≥50 ppm). The incidence of LGLL was not significantly increased in the treated males compared to the controls. No other treatment-related increased incidence of tumours was seen (Van Miller et al., 2002). [Kl. score = 2]

Male and female Wistar rats were given in their drinking water 0, 100, 500 or 2,000 ppm glutaraldehyde for two years. The mean daily intake of glutaraldehyde was as follows: 0, 6.1, 31.9 and 120.7 mg/kg-day for males; and 0, 10.5, 48.5 and 176.4 mg/kg-day for females. In the high-dose animals, there was mortality (2 males and 9 females) from asphyxia, and mean terminal body weights were significantly decreased compared to the controls. There were no treatment-related neoplastic effects (ECHA). [Kl. score = 1]

Inhalation

Male and female B6C3F_1 mice were exposed by inhalation to 0 or 0.1 ppm (0 or 0.4 mg/m^3) glutaraldehyde for 6 hours/day, 5 days/week for 52 and 78 weeks. No exposure-related neoplastic lesions were observed in either males or females (Zissu et al., 1998). [Kl. score = 2]

Male and female Fischer 344 rats were exposed by inhalation to 0, 0.25, 0.5 or 0.75 ppm (0, 1, 2 or 3.1 mg/m^3) glutaraldehyde for 6 hours/day, 5 days/week for two years. Survival in the mid- and high-dose females was statistically significantly decreased compared to controls. Survival of the treated males was similar to controls. No exposure-related neoplastic lesions were observed in either males or females (van Birgelen et al., 2000). [Kl. score = 2]

Male and female B6C3F_1 mice were exposed by inhalation to 0, 0.0625, 0.125 or 0.25 ppm (0, 0.26, 0.5 or 1 mg/m^3) glutaraldehyde for 6 hours/day, 5 days/week for two years. Survival of the treated animals was similar to controls. No exposure-related neoplastic lesions were observed in either males or females (van Birgelen et al., 2000). [Kl. score = 2]

I. Reproductive Toxicity

A two-generation reproductive toxicity study was conducted in Wistar rats given 0, 100, 500 and 2000 ppm glutaraldehyde in their drinking water. The approximately mean daily intake is 0, 12, 58 and 199 mg/kg-day for the parental males and females of the F_0 and F_1 generation during pre-mating. There were no adverse effects on reproductive performance or fertility. Oestrous cycle data, mating behaviour, conception, gestation, parturition, lactation and weaning as well as sperm parameters, sexual organ weights, gross and histopathological findings of these organs were similar between treated and control groups. In the high-dose animals, there was decreased water and/or food consumption; and decreased body weights and/or reduced body weight gains during the pre-mating periods in the F_0 and F_1 parental females during pre-mating, gestation and/or lactation. The

high-dose F_1 parental females also had increased the number of erosions/ulcers with microscopic erosion(s) or inflammatory oedema in the mucosa/submucosa of the glandular stomach. There were no adverse effects in the 500 ppm animals except for slight decreases in water consumption due to a palatability (bad taste) problem. Treatment-related signs of developmental toxicity were seen in the progeny of the high-dose F_0 and F_1 parental generation, and included impairment in body weight and consequently in organ weights in the respective F_1 and F_2 pups. The NOAEL for reproductive toxicity is 2,000 ppm (199 mg/kg-day), the highest dose tested. The NOAEL for parental systemic toxicity is 500 ppm (58 mg/kg-day). The NOAEL for developmental toxicity is 500 ppm or 58 mg/kg-day (ECHA). [Kl. score = 1]

A two-generation reproductive toxicity study was conducted in Crj: CD(SD) rats given 0, 50, 250 and 1,000 ppm glutaraldehyde in their drinking water. Mean daily intake was not calculated. Parental body weights and body weight gains were significantly reduced at 1,000 ppm at some periods, particularly during pre-mating. Food consumption was significantly reduced at 1,000 ppm for the F_0 and F_1 parental animals during pre-mating and gestation, and F_1 females during lactation. Water consumption was reduced throughout the pre-mating period for the F_0 and F_1 250 and 1,000 ppm parental animals. There was no indication of adverse effects on reproductive performance or fertility at any dose level. For the F_1 1,000 ppm offspring, body weights were reduced from lactation days 21-28. The NOAEL for reproductive toxicity is 1,000 ppm, the highest dose tested. The NOAEL for parental systemic toxicity is 50 ppm. The NOAEL for developmental toxicity is 250 ppm (Neeper-Bradley and Ballantyne, 2000). [Kl. score = 2]

J. Developmental Toxicity

Pregnant Wistar rats were given in their drinking water 0, 50, 250 or 750 ppm (0, 5, 26 or 68 mg/kg) glutaraldehyde from GD 6 to 16. Water consumption was reduced in a dose-related manner in the $\geq$250 ppm dams, and was considered not to be a toxic response, but due to the palatability (bad taste) of the drinking test solution. No other maternal effects were seen in the study. There were no significant differences between treated and controls in the sex distribution, placental weights, foetal weights, malformations or variations. The NOAEL for maternal and developmental toxicity in this study is 68 mg/kg-day, respectively (ECHA). [Kl. score = 1]

Pregnant Wistar rats were dosed by oral gavage with 0, 25, 50 or 100 mg/kg glutaraldehyde on GD 6 to 15. Mortality was significantly increased in the high-dose group (5/26); there were 2/21 deaths in the mid-dose group. Clinical signs (piloerection) occurred in all treated groups in a dose-dependent manner. Maternal body weight gain and feed consumption were significantly reduced in the high-dose dams, but not at the lower doses. The necropsy findings showed evidence of stomach irritation in almost all of the animals that died during the study and in 12/21 of the surviving dams in the high-dose group. The number of implantation per litter, resorptions and dead foetuses per litter, live foetuses per litter and incidence of post-implantation loss per litter was similar across all groups. The mean foetal body weights for male and female foetuses were significantly reduced in the high-dose group; this was attributed to the reduced food consumption of the dams during gestation rather than a direct effect of treatment. There was no evidence of a treatment-related teratogenic effect. The NOAEL for maternal and developmental toxicity is 50 mg/kg-day, respectively (Ema et al., 1992). [Kl. score = 2]

Pregnant Himalayan rabbits were dosed by oral gavage with 0, 5, 15 or 45 mg/kg glutaraldehyde on GD 7 to 19. In the high-dose group, 5/15 died on GD 9-11. Food consumption and body weight gain

were also significantly reduced in the high-dose group. Clinical observations in 12/15 high-dose does included soft faces, diarrhoea and blood in the bedding. The mean gravid uterus weight was significantly reduced in the high-dose group. Post-implantation loss was greatly increased (94.3%) in the high-dose group: no viable foetuses in 9/15 of the high-dose does, only early resorptions; only one female gave four alive foetuses on the scheduled date. There were reduced placental and foetal body weights in the only four foetuses. No significant maternal or developmental effects were seen in the mid- and low-dose groups. The NOAEL for maternal and developmental toxicity in this study is 15 mg/kg-day (ECHA). [Kl. Score = 2]

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for glutaraldehyde follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

The lowest NOAEL values from key toxicity studies on glutaraldehyde are listed in Table 7.

Table 7 Lowest NOAEL Values from Key Toxicity Studies on Glutaraldehyde by the Oral Route

Species/Sex	Study Duration	mg/kg-day	Endpoint	Reference
Rats, female	90-days	4	Decreased body weights, food and water consumption	ECHA
Rats, male	13-wk (drinking water)	5	Increased kidney weights	ECHA
Rats, male	12-months (drinking water)	30.5	Clinical signs; decreased body weights and food consumption; increased clear cell foci in liver	ECHA
Rats, male	2-yr (drinking water)	4	Reduced body weight, body-weight gain, and food consumption	Van Miller *et al.* (2002)
Rats	2-generation (drinking water)	58	Systemic toxicity	ECHA
Rats	GD 6-16 (drinking water)	68	Developmental toxicity	ECHA
Rats	GD 6-15 (oral gavage)	50	Developmental toxicity	Ema *et al.* (1992)
Rabbits	GD 7-19 (oral gavage)	15	Developmental toxicity	ECHA

The lowest NOAEL from these studies is 4 mg/kg-day based on reduced body weights, body weight gain, and feed consumption in male rats from the two-year drinking water study (Van Miller et al., 2002). The NOAEL of 4 mg/kg-day will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 4/(10 x 10 x 1 x 1 x 1) = 4/100 = 0.04 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD: Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2 L (ADWG, 2011)

Drinking water guidance value = (0.04 x 70 x 0.1)/2 = 0.14 mg/L

Cancer

Increased incidence of large granular cell lymphatic leukaemia (LGLL) was observed in all groups of male and female Fischer 344 rats given glutaraldehyde in their drinking water, including the controls (Van Miller *et al.* 2002). For the males, the incidence of LGLL was not statistically significantly increased. However, for the females, the incidence of LGLL was significantly increased in all treated females (≥50 ppm). Inhalation exposure of Fischer 344 rats to glutaraldehyde did not result in an increased incidence of tumours, including LGLL.

LGLL, also known as mononuclear cell leukaemia, is an extremely common spontaneous neoplastic disease of the ageing F344 rat (Stromberg, 1985; Ward *et al.,* 1990; Thomas et al. 2007). Consistent features are splenomegaly, anaemia, thrombocytopenia and leukemic infiltration of the spleen, liver lung, and in an advanced stage, of several other organs. The incidence is variable but has been increasing progressively with time and can exceed 70% in controls in some studies. This compares

with background incidence of less than 1% in other strains of commonly used laboratory rats (Haseman et al., 1998; Thomas et al., 2007). The incidence in F344 rats is modulated by a variety of factors not clearly related to carcinogenicity. Corn oil gavage, for example, has been shown consistently to reduce the incidence of MCL in male, but not female, controls (reviewed in Thomas et al., 2007).

The neoplastic mononuclear cells appear to be derived from large granular lymphocytes (LULs) (reviewed in Thomas et al., 2007). The tumour cell is of the NK type in most, if not all, cases. LGLL, although uncommon, does occur in humans. There are two types: T-LGLL which has a chronic course characterised by neutropenia, recurrent infections, splenomegaly and accompanying rheumatoid arthritis, and the much rarer NK-LGLL which has an acute course, more pronounced splenomegaly, and thrombocytopenia. The latter type appears to resemble more closely the disease in the F344 rat than the former. The aetiology of human LGLL is unknown. There is some evidence that viral infection may play a role but no evidence that a chemically-related increased of LGLL in the F344 rat is indicative of the potential to induce LGLL in humans.

To extrapolate results from an animal model that has a clear predisposition (high spontaneous rates) to a tumour type to humans, of which this is not the case, seems inappropriate if the mechanism(s) for LGLL formation in that strain is not understood. Although that rat strain may be useful for understanding the disease process in humans, it does not seem reasonable to use the results from that rat strain for risk assessment purposes. There should be confirmation of a putative leukemogenic effect in the F344 rat in another strain before any conclusions are made about the use of this tumour type for human health risk assessment purposes.

L. Human Health Hazard Assessment of Physico-Chemical Properties

Glutaraldehyde does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Glutaraldehyde has a moderate acute toxicity concern to fish and invertebrates, but is highly toxic to algae. It is of low toxicity concern to terrestrial invertebrates and plants. To birds, glutaraldehyde is moderately toxic on an acute basis and slightly toxic on a subacute dietary basis.

B. Aquatic Toxicity

Acute Studies

Table 8 lists the results of acute aquatic toxicity studies conducted on glutaraldehyde.

Table 8 Acute Aquatic Toxicity Studies on Glutaraldehyde

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Bluegill sunfish	96-hr LC_{50}	13	2	ECHA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Oncorhynchus mykiss	96-hr LC_{50}	10	2	ECHA
Daphnia magna	48-hr LC_{50}	14.87	2	ECHA
Daphnia magna	48-hr LC_{50}	14	2	ECHA
Scenedesmus subspicatus	72-hr EC_{50}	0.375 (biomass) 0.6 (growth rate) 0.025 (NOEC)	1	ECHA
Scenedesmus subspicatus	72-hr EC_{50}	0.92 (growth rate) 0.61(biomass) 0.33 (NOEC)	2	ECHA; Leung, 2001
Scenedesmus subspicatus	72-hr EC_{50}	0.61 (growth rate)	2	ECHA

Chronic Studies

The chronic aquatic toxicity studies conducted on glutaraldehyde are listed in Table 9.

Table 9 Chronic Aquatic Toxicity Studies on Glutaraldehyde

Test Species	Endpoint	Results (mg/L)	Kl. score	Reference
Oncorhynchus mykiss	97-day (OECD 210)	LOEC = 5 NOEC = 1.6	1	ECHA
Daphnia magna	21-day	NOEC = 5	1	ECHA

C. Terrestrial Toxicity

Table 10 lists the results of toxicity studies conducted on glutaraldehyde with earthworms, soil microorganisms and birds.

Table 10 Terrestrial Toxicity Studies on Glutaraldehyde

Test Species (method)	Endpoint	Results	Kl. score	Reference
Earthworm *Eisenia fetida* (OECD 207)	14-d LC_{50}	>500 mg/kg soil dw	1	ECHA
Soil microorganisms* (OECD 216)	28-d EC_{50} 28-d EC_{10}	360 mg/kg soil dw 11.5 mg/kg soil dw	1	ECHA
Soil microorganisms* (OECD 217)	28-d EC_{50} 28-d EC_{10}	>593 mg/kg soil dw 1.5 mg/kg soil dw	1	ECHA
Mallard ducks	Single-dose (oral gavage) LC_{50}	206 mg/kg	2	ECHA
Mallard ducks	5-d (dietary) NOEC	>2,500 ppm	1	ECHA

*organic carbon content of soil = 1.34% dry weight

Glutaraldehyde has also been evaluated in a terrestrial plants test: seedling emergence and seedling growth test (OECD TG 208). The test material contained 48.9% glutaraldehyde. The results are as follows:

Avena sativa (oats): 19-day EC_{50} value is >1,000 mg/kg soil dry weight based on emergence rate, dry weight and shoot length. The NOECs for *Avena sativa* (oats) were ≥1,000 mg/kg dry weight on all three parameters tested

Brassica napus (rapeseed): 19-day EC_{50} is >1,000 mg/kg soil dry weight based on emergence rate and shoot length and 994 mg/kg soil dry weight based on dry weight. The NOECs were ≥1,000, 500, and 250 mg/kg soil dry weight for emergence rate, dry matter and shoot length, respectively.

Vicia sativa (vetch): 19-day EC_{50} is >1,000 mg/kg soil dry weight based on emergence rate and shoot length, and 901 mg/kg soil dry weight based on dry weight. The NOECs were ≥1,000, 125, and 125 mg/kg soil dry weight for emergence rate, dry matter, and shoot length, respectively (ECHA). [Kl. score = 1]

D. Calculation of PNEC

The PNEC calculations for glutaraldehyde follow the methodology discussed in DEWHA (2009).

PNECwater

Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (10 mg/L), *Daphnia* (14 mg/L) and algae (0.375 mg/L). Results from chronic studies are also available for all three trophic levels, with the lowest NOEC being 0.025 mg/L for algae. On the basis that the data consists of short-term and long-term results from three trophic levels, an assessment factor of 10 has been applied to the lowest reported NOEC of 0.025 mg/L for algae. The $PNEC_{water}$ is 0.0025 mg/L.

PNECsediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.006 mg/kg wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (3.1/1280) \times 1000 \times 0.0025$
$= 0.006$

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 4.8)/1000 \times 2400]$
$= 3.1$

Where:

Kp_{sed} = solid-water partition coefficient (L/kg)

BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{0c} \times f_{oc}$
= 120 x 0.04
= 4.8

Where:

K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for glutaraldehyde in sediment is 120

F_{oc} = fraction of organic carbon suspended sediment = 0.04 [default]

PNECsoil

Experimental results are available for three trophic level. An acute LC_{50} value is available for earthworms (>500 mg/kg). Results from long-term studies are available for two trophic levels, with the lowest NOEC or EC_{10} being 1.5 mg/kg soil dry weight for soil organisms.

The EC_{10} value is corrected for bioavailability of glutaraldehyde in soil by normalising to the fraction organic carbon matter content (Fom) in the soil using the following equation:

$EC_{10(std)} = EC_{10(exp)} \times Fom_{soil(std)}/Fom_{soil(exp)}$

Where:

$Fom_{soil(std)}$ = 1% (default soil fraction organic matter)

$Fom_{soil(exp)}$ = 1.34% (see Table 10)

$EC_{10(std)}$ = 1.5 mg/kg x 1/1.34 = 1.12 mg/kg

On the basis that the data consists of one short-term from one trophic level and two long-term results from two additional levels, an assessment factor of 50 has been applied to the lowest reported long-term EC_{10} of 1.12 mg/kg soil dry weight [corrected for organic carbon content] for soil organisms. The $PNEC_{soil}$ is 0.02 mg/kg soil dry weight.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Glutaraldehyde is readily biodegradable and thus does not meet the screening criteria for persistence.

The log K_{ow} for glutaraldehyde at different pH values ranges from -0.36 to -0.80. Thus, glutaraldehyde does not meet the screening criteria for bioaccumulation.

The lowest NOEC value from chronic aquatic toxicity studies is <0.1 mg/L. Thus, glutaraldehyde meets the screening criteria for toxicity.

The overall conclusion is that glutaraldehyde is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, glutaraldehyde does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for glutaraldehyde.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Glutaraldehyde	111-30-8	Not a PBT	No	No	No	No	No	Yes	2 (fish & invertebrates) 3 (algae)	2	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
ALT	alanine aminotransferase

AST	aspartate aminotransferase
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
dw	dry weight
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
GD	gestation day
HHRA	enHealth Human Risk Assessment
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilogrammes per cubic metre
Kl	Klimisch scoring system
kPa	kilo pascal
L	litre
LC	lethal concentration
LD	lethal dose
LGLL	large granular lymphocytic leukaemia
LOAEL	lowest observed adverse effect level
LOEC	lowest observed effect concentration
LUL	large granular lymphocyte
MCL	maximum contaminant level
mg/cm^2	milligrams per square centimetre
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mm^2/s	square millimetres per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NK	natural killer
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development

Pa m^3/mol	pascal meter squared per gram molecular weight
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SCE	sister chromatid exchange
SGG	Synthetic Greenhouse Gases
SIDS	Screening Information Data Set
SLRL	sex-linked recessive lethal
TG	Test Guideline
UDS	Unscheduled DNA Synthesis

Attachment 3 Risk Characterisation Tables

Attachment 3, Table 1
Summary of Exposure Point Concentrations

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)[1]	Estimated Concentration in Combined Balance Water Feed Pond to WMF (mg/L)[2]		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[3]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[4]		Estimated Concentration in Dawson River Sediment (mg/kg)[5]	
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)	
					0	30	0	30	0	30	0	30
Glutaraldehyde	111-30-8	8.00E-04	1.50E+01	1.07E-04	1.07E-05	2.67E-06	1.07E-07	2.67E-08	2.13E-09	5.33E-10	5.17E-09	1.29E-09

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated flowback concentration in pond influent (150% of injected fluid volume) per coal seam per 20% of mass returned calculated using equation: Pond Influent = FBconcentration (mg/L)/ FB dilution 150% x percent mass returned (mg/L)
2) Estimated flowback concentration was multiplied by a factor of 10% to account for dilution in the water feed pond (90:1) due to the aggregation of produced water from other wells which were not recently hydraulically fractured into the same pond.
3) Concentrations in the water feed pond were further reduced by a factor of 99% to account for efficiencies in the WMF system.
4) A dilution factor of 50 was assumed within the approved mixing zone.
5) $EPC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times EPC_{water}$
Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = treated water EPC
$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]
$Kp_{sed} = K_{oc} \times f_{oc}$
Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg), chemical-specific value found in dossier provided in Attachment 1.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

Attachment 3, Table 2
Comparison of Theoretical Concentrations of COPCs to Drinking Water Guidelines

Permeate Pond								
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[1]		Drinking Water Screening Level (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30
Glutaraldehyde	111-30-8	1.07E-07	2.67E-08	2.13E-09	5.33E-10	1.40E-01	1.5E-08	3.8E-09

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 3, Table 3
Comparison of Theoretical Concentrations of COPCs to PNECs (Water and Sediment)

Permeate Pond													
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[1]		PNEC aquatic (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)		Estimated Concentration in Dawson River Sediment (mg/kg)[1]		PNEC sediment (mg/kg)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30	0	30		0	30
Glutaraldehyde	111-30-8	1.07E-07	2.67E-08	2.13E-09	5.33E-10	2.50E-03	8.53E-07	2.13E-07	5.17E-09	1.29E-09	5.40E-03	9.6E-07	2.4E-07

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 3, Table 4
Risk Estimates for Cattle Egret - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Avian NOAELt [1]	Avian NOAEL Test Animal		Avian Receptor Cattle Egret	
			Animal	Body Weight (kg)		Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Glutaraldehyde	111-30-8	4.00E+00	Rat	3.50E-01	2.06E+00	Mallard Duck	1.58E+00	3.90E-01	2.9E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ Avian NOAEL for gluteraldehyde developed by applying an uncertainty factor of 100 to the LD50 for mallard duck.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.03	(c)
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	0.39	Siegfried, 1969
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
W.R. Siegfried (1969) Energy Metabolism of the Cattle Egret, ZoologicaAfricana, 4:2, 265-273, DOI: 10.1080/00445096.1969.11447375
c/ Drinking water ingestion rate (WIR) based on the allometric relationship developed by Calder and Braun (1983), where WIR (L/day) = 0.059 x BW (Kg)$^{0.67}$

Constituent Name	CAS No.	EPC [1] Day 0	EPC [1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Glutaraldehyde	111-30-8	2.1E-09	5.3E-10	2.9E+00	3.1E-12	1.1E-12	7.9E-13	2.7E-13

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365^{\ days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 3, Table 5
Risk Estimates for Kangaroo - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Mammal Kangaroo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Glutaraldehyde	111-30-8	4.00E+00	Rat	3.50E-01	2.50E+01	1.38E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weight test}{Body\ Weight receptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	3	Fleming, 2001
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	25	Fleming, 2001
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
Fleming, 2001
Fleming, Peter; Laurie Corbett, Robert Harden, Peter Thomson (2001). Managing the Impacts of Dingoes and Other Wild Dogs. Commonwealth of Australia: Bureau of Rural Sciences.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Glutaraldehyde	111-30-8	2.1E-09	5.3E-10	1.4E+00	4.9E-12	3.6E-12	1.2E-12	8.9E-13

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 3, Table 6
Risk Estimates for Dingo - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Dingo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Glutaraldehyde	111-30-8	4.00E+00	Rat	3.50E-01	1.30E+01	1.62E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.75	Dawson, 1995
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	13	Dawson, 1995
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
Dawson, 1995
Dawson, Terence J. (1995). Kangaroos: Biology of the Largest Marsupials. Cornell University Press, Ithaca, New York. Second printing: 1998. ISBN 0-8014-8262-3.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Glutaraldehyde	111-30-8	2.1E-09	5.3E-10	1.6E+00	2.4E-12	1.5E-12	5.9E-13	3.6E-13

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 3, Table 7
Risk Estimates for Cattle - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Cattle	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Glutaraldehyde	111-30-8	4.00E+00	Rat	3.50E-01	4.54E+02	6.67E-01

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weight test}{Body\ Weight receptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	86	API, 2004
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	454	API, 2004
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
API, 2004
API. (2004). Risk-Based Screening Levels for the Protection of Livestock Exposed to Petroleum Hydrocarbons, Regulatory Analysis and Scientific Affairs No. 4733 July 2004.

Constituent Name	CAS No.	EPC [1] Day 0	EPC [1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Glutaraldehyde	111-30-8	2.1E-09	5.3E-10	6.7E-01	7.8E-12	1.2E-11	1.9E-12	2.9E-12

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Qualitative and Quantitative Tier 3 Assessment

Hydrochloric Acid

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Hydrochloric acid is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to improve formation permeability, enhancing the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Hydrochloric acid	7647-01-0	pH correction	0.0776%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. Repeated dose, reproductive and developmental toxicity studies by the oral route have not been conducted on hydrochloric acid. These toxicity studies would have questionable usefulness because of the corrosive/irritating nature of hydrochloric acid, which would limit the amount of absorbed HCl. Hydrochloric acid dissociates to hydrogen (H^+) and chloride (Cl^-) ions in bodily fluids, and a significant amount of these ions are already ingested in foods. Furthermore, both ions are present in the body and are highly regulated by homeostatic mechanisms. Therefore, an oral reference dose (RfD) and drinking water guideline value were not derived for hydrochloric acid.

Australian Drinking Water Guideline (ADWG) value for pH and chloride (see **Table 2**) may be applicable.

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Hydrochloric acid (7647-01-0)	pH; chloride	6.5 to 8.5; 250 mg/L (aesthetics)

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicity reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

PNEC values were not derived for hydrochloric acid because factors such as the buffer capacity, the natural pH, and the fluctuation of the pH are very specific for a certain ecosystem. Refer to **Attachment 1** for additional rationale.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Hydrochloric acid can exist in a gaseous phase at room temperature and pressure. Hydrochloric acid is also very soluble in water and is a strong acid that dissociates completely in water to hydrogen (H^+) and chloride (Cl^-) ions. Both ions are ubiquitous in the environment. The molecular structure of hydrochloric acid is presented in **Figure 1**.

Figure 1 Molecular Structure of Hydrochloric Acid[2]

The addition of hydrochloric acid to an aquatic ecosystem could potentially increase the chloride concentration and may decrease the pH depending on the buffer capacity of the receiving water. H^+ and Cl^- ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for hydrochloric acid is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that hydrochloric acid is not a PBT substance.

Human Health Hazards

Hydrochloric acid is a corrosive liquid. Depending on the concentration, aqueous solutions of hydrochloric acid are either corrosive, irritating or non-irritating to the skin, eyes and gastrointestinal tract. Vapours from aqueous solutions of hydrochloric acid can cause respiratory irritation. Hydrochloric acid is not a skin sensitiser.

No repeated dose toxicity studies have been conducted by the oral route. Subchronic inhalation studies show localised irritation to the upper respiratory tract of rats and mice, but no systemic toxicity. Positive findings have been reported in some *in vitro* genotoxicity studies, which are considered to be the result of the pH change in the test system. No adequate reproductive or developmental studies have been conducted on hydrochloric acid. Hydrochloric acid is not a carcinogen.

TRVs were not derived for hydrochloric acid. The ADWG values for pH (6.5 to 8.5) and chloride (250 mg/L, aesthetics) may be applicable.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently,

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/7647-01-0

there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the environmental fate properties described in **Attachment 1** and discussed above, hydrochloric acid dissociates completely in aqueous media to hydrogen (H^+) and chloride (Cl^-) ions. Both ions are ubiquitous in the environment. As a result, this chemical would not be present within the water feed pond. Likewise, during water treatment it would be removed by the reverse osmosis (RO) system, with the majority directed to brine (i.e., less than 5% to permeate). Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

National Industrial Chemicals Notification and Assessment Scheme (NICNAS) identified hydrochloric acid as a low concern for workers and the public under the operational scenarios assessed. Best practice chemical management was recommended to minimise worker and public exposure (NICNAS, 2017a).

Environmental Hazards

Hydrochloric acid is an inorganic salt that dissociates completely to hydrogen (H^+) and chloride (Cl^-) ions in aqueous solutions. The hazard of hydrochloric acid for aquatic organisms is caused by the hydrogen ion (H^+). The toxicity values in terms of mg/L are not relevant because of the varying buffering capacity of different test systems and different aquatic ecosystems.

Biodegradation is not applicable to these inorganic ions; both hydrogen (H^+) and chloride (Cl^-) ions are also ubiquitous and are present in water, soil and sediment. In addition, hydrogen (H^+) and chloride (Cl^-) ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Thus, hydrochloric acid is not expected to bioaccumulate.

In the aquatic environment, the toxicity of hydrochloric acid will be influenced by factors such as the buffer capacity, the natural pH, and pH fluctuation of the ecosystem. PNEC values for water were derived as part of NICNAS based on a chronic aquatic toxicity study. However, experimental details were not available to validate the PNEC. Terrestrial toxicity studies were also not available. Therefore, PNEC values for water, soil and sediment have not been derived. Based on its properties, hydrochloric acid is not expected to significantly adsorb to soil or sediment, and if released to the ground would be neutralised by the slightly alkaline environment of the earth (NICNAS, 2017b).

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

1. Aquatic ecological receptors within Dawson River downstream of the release point
2. Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released produced water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

In addition, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to hydrochloric acid that may occur during hydraulic fracturing and work over activities. The risk characterisation evaluates the toxicity of this chemical and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, exposure pathways associated with Dawson River discharge would be incomplete. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with chemicals used during stimulation activities is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 1**), hydrochloric acid does not meet the criteria for persistence or bioaccumulation. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 4** below provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 4 Evaluation of Uncertainty – Hydrochloric Acid

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in residual stimulation fluids were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
	differ than those presented in the risk assessment.		
Toxicity Assessment	Oral toxicological reference doses and drinking water guidance values were not derived for hydrochloric acid (which dissociates completely to hydrogen and chloride ions).	Low	Low potential to underestimate risk
Toxicity Assessment	PNEC water values were not derived for hydrochloric acid. The hazard for aquatic organisms is caused by the hydrogen ion (H^+). The toxicity values in terms of mg/L are not relevant because of the varying buffering capacity of different test systems and different aquatic ecosystems.	Low to Medium	Low to medium potential to underestimate or overestimate risk

References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019.

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Department of the Environment and Energy (DoEE). (2017). Exposure draft: Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction. Commonwealth of Australia, available at http://www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual

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NICNAS. (2017a) National assessment of chemicals associated with coal seam gas extraction in Australia, Technical report number 12- Human health hazards of chemicals associated with coal seam gas extraction in Australia: Attachment 5 – Hazard assessment sheets. Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

Attachment 1 Risk Assessment Dossier

HYDROCHLORIC ACID

This dossier on hydrochloric acid presents the most critical studies pertinent to the risk assessment of hydrochloric acid in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from OECD-SIDS documents (OECD, 2002a,b), and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Hydrochloric acid was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Hydrochloric acid was assessed as a tier 3 chemical for acute toxicity. Data were not available to categorize the substance based on chronic effects. Therefore, hydrochloric acid is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Hydrochloric acid (HCl) can exist in a gaseous phase at room temperature and pressure. Due to its high water solubility and low vapour pressure, hydrochloric acid will be found predominantly in the aquatic environment where it dissociates completely to hydrogen (H^+) and chloride (Cl^-) ions. Both ions are ubiquitous in the environment. H^+ and Cl^- ions will not adsorb on particulate matter or surfaces and will not accumulate in living tissues. Hydrochloric acid is a corrosive liquid. Depending on the concentration, aqueous solutions of hydrochloric acid (HCl) are either corrosive, irritating, or non-irritating to the skin, eyes and gastrointestinal tract. Vapours from aqueous solutions of HCl can cause respiratory irritation. HCl is not a skin sensitiser. Subchronic inhalation studies show localised irritation to the upper respiratory tract of rats and mice, but no systemic toxicity. No repeated dose toxicity studies have been conducted by the oral route. Positive findings have been reported in some in vitro genotoxicity studies, which are considered to be the result of the pH change in the test system. A lifetime inhalation study showed no carcinogenic effects in rats exposed to HCl. No adequate reproductive or developmental studies have been conducted on HCl. The hazard of hydrochloric acid for aquatic organisms is caused by the hydrogen ion (H^+). The toxicity values in terms of mg/L are not relevant because of the varying buffering capacity of different test systems and different aquatic ecosystems.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Chlorane

CAS RN: 7647-01-0

Molecular formula: HCl

Molecular weight: 36.46

Synonyms: Hydrochloric acid, HCl, chlorane, hydrogen chloride, muriatic acid, chlorohydric acid

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Hydrochloric Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless to slightly yellow gas of fuming liquid with pungent, irritating odour.	2	ECHA
Melting Point	-114.22°C	2	ECHA
Boiling Point	-85°C	4	ECHA
Density	1.639 g/L @ 0°C (gas) 1.194 g/mL @ 26°C (liquid)	4	ECHA
Vapour Pressure	4,104 kPa 4,723 kPa @ 25°C	4	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	Very soluble	4	ECHA
Viscosity	1.7 x 10^{-6} m^2s @ 20°C	1	ECHA

Hydrochloric acid can exist in a gaseous phase at room temperature and pressure. Hydrochloric acid is also very soluble in water and is a strong acid that dissociates completely in water to hydrogen (H^+) and chloride (Cl^-) ions.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No other specific environmental regulatory controls or concerns were identified within Australia and internationally for hydrochloric acid.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Due to its high water solubility, hydrochloric acid will be found predominantly in the aquatic environment where it dissociates completely to hydrogen (H^+) and chloride (Cl^-) ions. Both ions are ubiquitous in the environment (UNEP, 1995).

The addition of hydrochloric acid to an aquatic ecosystem may decrease the pH depending on the buffer capacity of the receiving water. In general, the buffer capacity is regulated by the equilibria between CO_2, HCO_3^- and CO_3^{2-}:

$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$ ($pKa_1 = 6.35$)

$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ ($pKa_2 = 10.33$)

A release of hydrochloric acid into the aquatic environment from the use of HCl could potentially increase the chloride concentration and decrease the pH in the aquatic environment. Table 3 shows the amount of hydrochloric acid that would need to be added to bicarbonate solutions to obtain pH values of 6.0 and 4.0. The UNEP (1995) study reported that the 10th percentile, mean and the 90th percentile of bicarbonate concentrations in 77 rivers in North America, South America, Asia, Africa, Europe and Oceania were 20, 106 and 195 mg/L, respectively. The data show that the decrease in pH depends on the buffering capacity (bicarbonate concentration) of the receiving water. The calculated values in Table 3 were confirmed experimentally.

Table 3 Buffer capacity to maintain the pH based on bicarbonate concentration from UNEP monitoring data (de Groot and van Dijk, 2002; taken from OECD, 2002b)

Initial concentration of HCO_3^-	Final pH	Concentration of HCl required to obtain the final pH value
		Calculated [mg/L]
20 mg/L HCO_3^- (10th percentile 77 rivers)	6.0	8.28
	4.0	11.9
106 mg/L HCO_3^- (mean value of 77 rivers)	6.0	43.9
	4.0	63.2
195 mg/L HCO_3^- (90th percentile 77 rivers)	6.0	80.7
	4.0	116.3

H^+ and Cl^- ions will not adsorb on the particulate matter or surfaces and will not accumulate in living tissues (OECD, 2002a,b).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Hydrochloric acid is a corrosive liquid. Depending on the concentration, aqueous solutions of hydrochloric acid (HCl) are either corrosive, irritating, or non-irritating to the skin, eyes and gastrointestinal tract. Vapours from aqueous solutions of HCl can cause respiratory irritation. HCl is not a skin sensitiser. Subchronic inhalation studies show localised irritation to the upper respiratory tract of rats and mice, but no systemic toxicity. No repeated dose toxicity studies have been conducted by the oral route. Positive findings have been reported in some *in vitro* genotoxicity studies, which are considered to be the result of the pH change in the test system. A lifetime inhalation study showed no carcinogenicity in rats exposed to HCl. No adequate reproductive or developmental studies have been conducted on HCl.

B. Acute Toxicity

The oral LD_{50} values in rats were reported to be 238 to 277 mg/kg and 700 mg/kg (OECD, 2002a,b). [Kl. scores = 2 and 4, respectively]

The lethal dose by dermal exposure is >5,010 mg/kg for rabbits (OECD 2002a,b). [Kl. score = 4]

The LC_{50} values in rats for HCl gas are 40,989 and 4,701 ppm for 5 and 30 minutes, respectively (ECHA) [Kl. score = 2]. The LC_{50} values in rats for HCl aerosol are 31,008 and 5,666 ppm (45.6 and 8.3 mg/L) for 5 and 30 minutes, respectively (ECHA). [Kl. score = 2]

C. Irritation

Application of a 37% aqueous solution of HCl for 1 or 4 hours was corrosive to the skin of rabbits (OECD, 2002a,b) [Kl. score = 2). Application of 0.5 mL of a 17% solution of aqueous solution of HCl for 4 hours was corrosive to the skin of rabbits (OECD, 2002a,b) [Kl. score = 3]. Moderate skin irritation was observed in rabbits following an application of 0.5 mL of a 3.3% aqueous solution of HCl for five days; no irritation was observed with 0.5 mL of a 1% aqueous solution (OECD, 2002a,b) [Kl. score = 2]. In humans, an aqueous solution of 4% of HCl was slightly irritating, while a 10% solution was sufficiently irritating to be classified as a skin irritant (OECD, 2002a,b).

Instillation of 0.1 mL of a 10% aqueous solution of HCl to the eyes of rabbits resulted in severe eye irritation (ECHA) [Kl. score = 2]. Instillation of 0.1 mL of a 5% solution of HCl produced corneal opacity, iridial lesions, conjunctival redness and chemosis in 3/3 animals at 1 hour and at day 1 post-instillation. There was no recovery in any animal and the study was terminated on day 2 (ECHA). [Kl. score = 1]

D. Sensitisation

Hydrochloric acid was not a skin sensitiser in a guinea pig maximisation test (ECHA). [Kl. score = 2]

E. Repeated Dose Toxicity

Oral

No adequate studies were located.

Inhalation

Male and female SD rats and F344 rats were exposed by inhalation to 0, 10, 20 or 50 ppm 6 hours/day, 5 days/week for up to 90 days. Clinical signs were mainly indicative of the irritant/corrosive nature of HCl. Body weights were significantly decreased in the 50 ppm male F344 rats. There were no treatment-related effects on the haematology or clinical chemistry parameters or urinalysis. At study termination, heart, kidney and testes weights were increased in the 100 and/or 50 ppm groups; these changes were considered to be mainly related to the treatment-related effect on body weight. Histopathological examination showed minimal to mild rhinitis in the ≥20 ppm dose groups of both strains of rats (both sexes). The NOAELs for systemic toxicity and localised irritation (site-of-contact) are 20 and 10 ppm, respectively (ECHA). [Kl. score = 1]

Male and female B6C3F_1 mice were exposed by inhalation to 0, 10, 20 or 50 ppm HCl, 6 hours/day, 5 days/week for up to 90 days. Clinical signs were mainly indicative of the irritant/corrosive nature of HCl. Body weights were significantly decreased in the 50 ppm groups. At study termination, absolute liver weights were decreased in the 50 ppm males. Histopathologic examination showed only eosinophilic globules in the nasal epithelium in the 50 ppm animals. The NOAEL for this study is 20 ppm (ECHA). [Kl. score = 1]

Male SD rats were exposed by inhalation to 0 or 10 ppm HCl 6 hours/day, 5 days/week for 128 weeks. Survival and body weights were similar between treated and control groups. There was a higher incidence of hyperplasia of the larynx compared to control, but no serious irritating effects of the nasal epithelium (ECHA). [Kl. score = 2]

Dermal

No studies were located.

F. Genotoxicity

In Vitro Studies

Table 4 presents the *in vitro* genotoxicity studies on hydrochloric acid.

Table 4 In Vitro Genotoxicity Studies on Hydrochloric Acid

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* and *E. coli* strains)	-	-	2	ECHA
Mammalian cell gene mutation (mouse lymphoma L5178Y cells)	-	+	2	ECHA
Chromosomal aberration (CHO cells)	+	+	2	ECHA

Test System	Results*		Klimisch Score	Reference
Saccharomyces cerevisiae (mitotic recombination	-	-	2	ECHA
E. coli W3110 (pol A+) and P3078 (pol A-) repair assay	-	-	2	ECHA

*+, positive; -, negative

In the mouse lymphoma assay, the mutant frequency increased as the pH was lowered to 6.5 to 6.0 (from increased HCl) in the presence of metabolic activation. A decrease in pH from the addition of HCl to the medium also resulted in clastogenic effects to CHO cells in the absence or presence of metabolic activation. The positive findings in these two studies are considered to be the result of the pH change in the test media.

In Vivo Studies

No adequate studies were located.

G. Carcinogenicity

Oral

No studies were located.

Inhalation

Male SD rats were exposed by inhalation to 0 or 10 ppm HCl 6 hours/day, 5 days/week for 128 weeks. Survival and body weights were similar between treated and control groups. There was a higher incidence of hyperplasia of the larynx compared to control, but no serious irritating effects of the nasal epithelium. There was no increased incidence of tumours in the HCl-treated rats compared to controls (ECHA). [Kl. score = 2]

H. Reproductive Toxicity

No studies were located.

I. Developmental Toxicity

No adequate studies were located.

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

Repeated dose, reproductive, and developmental toxicity studies by the oral route have not been conducted on hydrochloric acid. These toxicity studies would have questionable usefulness because of the corrosive/irritating nature of hydrochloric acid, which would limit the amount of absorbed HCl. Hydrochloric acid dissociates to hydrogen and chloride ions in bodily fluids, and a significant amount of these ions are already ingested in foods. Furthermore, both ions are present in the body and are highly regulated by homeostatic mechanisms. Thus, an oral toxicological reference and drinking water guidance values were not derived from hydrochloric acid.

The Australian drinking water guideline values for pH (6.5 to 8.5) and chloride (250 ppm, aesthetics) may be applicable (ADWG, 2011).

K. Human Health Hazard Assessment of Physico-Chemical Properties

Hydrochloric acid does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The hazard of hydrochloric acid for aquatic organisms is caused by the hydrogen ion (H^+). The toxicity values in terms of mg/L are not relevant because of the varying buffering capacity of different test systems and different aquatic ecosystems.

B. Aquatic Toxicity

Acute Studies

The acute aquatic toxicity studies on hydrochloric acid are listed in Table 5.

Table 5 Acute Aquatic Toxicity Studies on Hydrochloric Acid

Test Species	Endpoint	Results	Klimisch score	Reference
Lepomis macrochirus	96-hr LC_{50}	pH 3.25 – 3.5 (20mg/L)	2	ECHA; OECD 2002a,b
Daphnia magna	48-hr EC_{50}	pH 4.92 (0.45 mg/L)	1	ECHA
Chlorella vulgaris	72-hr EC_{50} 72-hr EC_{10}	pH 4.7 [growth rate](0.73 mg/L) PH 4.7 (0.364 mg/L)	1	ECHA

Chronic Studies

No chronic studies are available.

C. Terrestrial Toxicity

No studies are available.

D. Calculation of PNEC

PNEC values[1] were not derived for hydrochloric acid because factors such as the buffer capacity, the natural pH, and the fluctuation of the pH are very specific for a certain ecosystem.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Hydrochloric acid is an inorganic salt that dissociates completely to hydrogen and chloride ions in aqueous solutions. Biodegradation is not applicable to these inorganic ions; both hydrogen and chloride ions are also ubiquitous and are present in water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

Hydrogen and chloride ions are essential to all living organisms, and their intracellular and extracellular concentrations are actively regulated. Thus, hydrochloric acid is not expected to bioaccumulate.

No chronic toxicity data exist on hydrochloric acid. The acute EC_{50} values are >1 mg/L in fish, < 1 mg/L for invertebrates and algae. Thus, hydrochloric acid meets the screening criteria for toxicity.

The overall conclusion is that hydrochloric acid is a PBT substance based on toxicity to invertebrates and algae.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, hydrochloric acid does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for hydrochloric acid.

[1] An aquatic PNEC (mg/L) has been derived as part of the chemical assessment conducted under National Industrial Chemicals Notification and Assessment Scheme (NICNAS). However, the chronic aquatic toxicity data set used to derive the PNEC value was not available for review.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Hydrochloric Acid	7647-01-0	Not a PBT	No	No	NA	No	No	No	1 (fish) 3 (algae & inverts) (ECHA)	No data	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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OECD. (2002b). Screening Information Dataset (SIDS) Initial Assessment Report for Hydrogen chloride (CAS No. 7647-01-0), UNEP Publications.

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
CHO	Chinese hamster ovary
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency

EU	European Union
g/L	grams per litre
g/mL	grams per millilitre
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
kPa	kPa
LC	lethal concentration
LD	lethal dose
m^2s	square metres per second
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases

Qualitative and Quantitative Tier 3 Assessment

Peroxyacetic Acid

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Peroxyacetic acid is a component in a Water Management Facility (WMF) product used for membrane cleaning during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals – Tier 3 Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Hydrogen peroxide Acetic Acid Peroyxacetic Acid Water	7722-84-1 64-19-7 79-21-0 7732-18-5	Membrane cleaning	2 x 1000 L (IBC)

CAS No = Chemical Abstracts Service Number
CIP = clean-in-place
IBC = intermediate bulk container
L = litre

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Peroxyacetic acid is not a carcinogen; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Peroxyacetic Acid (79-21-0)	90-day rat oral gavage	Mortality, clinical signs, reduced body weights	23.4	300	0.08	0.3

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 2** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna for the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Peroxyacetic acid (79-21-0)	Acute fish	0.002	10	0.0002

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Peroxyacetic acid (79-21-0)	[a]	-	-	0.00013

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Peroxyacetic acid (79-21-0)	Terrestrial plant toxicity	180	50	3.6

EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Peroxyacetic acid is an organic peroxide. It is not flammable under conditions where the liquid is open to the atmosphere. However, a sustained flame is possible in a closed system. Decomposition of peroxyacetic acid produces oxygen. A closed system prevents the release of oxygen, which in the presence of the acetic acid can sustain a flame. Thus, all the gases produced remain in the system and can burn. The molecular structure of peroxyacetic acid is presented in **Figure 1**.

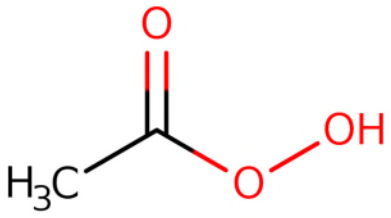

Figure 1 Molecular Structure of Peroxyacetic Acid[2]

Peroxyacetic acid will rapidly hydrolyse in water at high pH values (e.g., pH 9). It is readily biodegradable and is not expected to bioaccumulate. Thus, it has low potential to adsorb to sediment and soil.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for peroxyacetic acid is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that peroxyacetic acid is not a PBT substance.

Human Health Hazards

Peroxyacetic acid has high acute toxicity by the oral and inhalation routes and moderate toxicity by the dermal routes. Depending on the concentration, aqueous solutions of peroxyacetic acid are either corrosive, irritating or non-irritating to the skin, eyes and gastrointestinal tract. Vapours from aqueous solutions of peroxyacetic acid can cause respiratory irritation. It is not a skin sensitiser.

Repeated oral doses of peroxyacetic acid to rats showed no systemic toxicity. Peroxyacetic acid is not genotoxic. Developmental effects (but no teratogenicity) were seen in laboratory animals at oral doses that also were toxic to the pregnant females.

Based on a review of repeated dose and developmental toxicity studies, toxicological reference values were derived for peroxyacetic acid. The drinking water guideline value derived for peroxyacetic acid using the non-carcinogenic oral RfD is 0.3 mg/L.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/79-21-0

fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the treatment process described in **Attachment 1**, membrane cleaning waste is directed to the brine dams where peroxyacetic acid will rapidly break down. As a result, this chemical would not be present in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

In standard aquatic toxicity tests, peroxyacetic acid is highly toxic to aquatic organisms on both an acute and chronic basis. In the acute aquatic tests, algae were found to be the most sensitive species. Fish and *daphnia* were less susceptible. Acute terrestrial toxicity tests are available for earthworm, plants and soil microorganisms. Under typical environmental conditions, the chemical is expected to degrade rapidly in soil and water and does not persist in the environment. The chemical also does not bioaccumulate.

Experimental toxicity data on water and soil organisms was available for three trophic levels to calculate PNECs. However, there are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to peroxyacetic acid that may occur during water treatment activities. The risk characterisation evaluates the toxicity of peroxyacetic acid and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, peroxyacetic acid is not directed to the permeate or brine waste streams and would not be present in permeate, brine or treated water. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), peroxyacetic acid does not meet the criteria for persistence or bioaccumulation. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical

and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 6** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 6 Evaluation of Uncertainty – Peroxyacetic Acid

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in the water treatment process were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Hazard Assessment –COPC concentrations	Concentrations of COPCs evaluated in the quantitative risk assessment were assumed to be 100 percent of mass used in the water treatment process. This is a conservative assumption for chemicals that may degrade rapidly or volatilise.	Medium	This assumption may overestimate the calculated risks to receptors.
Toxicity Assessment	The absence of toxicity data for sediment-dwelling organisms to calculate a PNEC in sediment. The PNEC was calculated using the equilibrium partitioning method.	Medium	This assumption may overestimate risk.

References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019..

Australian Environmental Agency (AEA). (2009). Environmental Risk Assessment Guidance Manual for Industrial Chemicals, Commonwealth of Australia. Available: http://www.nepc.gov.au/resource/chemical-risk-assessment-guidance-manuals

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frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.

Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		On-site Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Hydrex 4714 (CIP)	Hydrogen Peroxide Acetic Acid Peroxyacetic Acid Water	7722-84-1 64-19-7 79-21-0 7732-18-5	20-30% 10-20% 5-10% n/a	Hydrex 4714	Veolia Water Solutions	Reverse Osmosis Plant	1000L IBC		2 x 1000L (IBC)		NIL		NIL	membrane cleaning

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
L/hr = litre per hour
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration
				(mg/L)	Permeate notes	(mg/kg)	(mg/kg)	(mg/L)
Hydrex 4714 (CIP)	Hydrogen Peroxide	7722-84-1	Membrane cleaning waste is directed to the Brine Dams	NA	This product is not directed to the permeate stream.	NA	NA	NA
	Acetic Acid	64-19-7		NA	This product is not directed to the permeate stream.	NA	NA	NA
	Peroxyacetic Acid	79-21-0		NA	This product is not directed to the permeate stream.	NA	NA	
	Water	7732-18-5		NA	This product is not directed to the permeate stream.	NA	NA	NA

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
L/hr = litre per hour
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Notes
Hydrex 4714 (CIP)	Hydrogen Peroxide	7722-84-1	all compounds break down, end up with water and carbon dioxide
	Acetic Acid	64-19-7	will biodgrade with in pond
	Peroxyacetic Acid	79-21-0	
	Water	7732-18-5	

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
L/hr = litre per hour
mg/kg = milograms per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

PEROXYACETIC ACID

This dossier on peroxyacetic acid presents the most critical studies pertinent to the risk assessment of peroxyacetic acid in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – Peroxyacetic acid was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Peroxyacetic acid was assessed as a tier 3 chemical for acute toxicity chronic toxicity. Therefore, peroxyacetic acid is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Peroxyacetic acid is an organic peroxide. It is not flammable under conditions where the liquid is open to the atmosphere. However, a sustained flame is possible in a closed system. Decomposition of peroxyacetic acid produces oxygen. A closed system prevents the release of oxygen, which in the presence of the acetic acid can sustain a flame. Thus, all the gases produced remain in the system and can burn. Peroxyacetic acid will rapidly hydrolyse in water at high pH values (e.g., pH 9). It is readily biodegradable and is not expected to bioaccumulate. It has low potential to adsorb to sediment and soil. Peroxyacetic acid has high acute toxicity by the oral and inhalation routes and moderate toxicity by the dermal routes. Depending on the concentration, aqueous solutions of peroxyacetic acid are either corrosive, irritating or non-irritating to the skin, eyes and gastrointestinal tract. Vapours from aqueous solutions of peroxyacetic acid can cause respiratory irritation. It is not a skin sensitiser. Repeated oral doses of peroxyacetic acid to rats showed no systemic toxicity. Peroxyacetic acid is not genotoxic. Developmental effects (but no teratogenicity) were seen in laboratory animals at oral doses that also were toxic to the pregnant females. Peroxyacetic acid is highly toxic to aquatic organisms on both an acute and chronic basis.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Ethaneperoxoic acid

CAS RN: 79-21-0

Molecular formula: $C_2H_4O_3$

Molecular weight: 76.1

Synonyms: Peroxyacetic acid; peracetic acid; ethaneperoxoic acid; acetic peroxide; peroxoacetic acid; monoperacetic acid; acetyl hydroperoxide

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Peroxyacetic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid	1	ECHA
Melting Point	-73°C (15.37% peroxyacetic acid; 25.56% hydrogen peroxide; 14.27% acetic acid)	1	ECHA
Boiling Point	105°C (15.37% peroxyacetic acid; 25.56% hydrogen peroxide; 14.27% acetic acid)	1	ECHA
Density	1.1284 g/cm^3	1	ECHA
Vapour Pressure	17 hPa @ 20°C	1	ECHA
Partition Coefficient (log K_{ow})	-0.59 @ 25°C (pH 5-9) [Experimental]	1	ECHA
Water Solubility	Very soluble	2	ECHA
Flash Point	>68 to <83°C	2	ECHA
Auto flammability	See below*	1	ECHA
pK_a	8.24	1	ECHA

*Most of the peroxyacetic acid equilibrium grades ranging from 5% to 15% exhibit only closed-cup flash points. Thus, these grades are not flammable under conditions where the liquid is open to the atmosphere. However, a sustained flame is possible in a closed system. Decomposition of peroxyacetic acid produces oxygen. A closed system prevents the release of the oxygen, which in the presence of the acetic acid can sustain a flame. Thus, all the gases produced remain in the system and they can burn. Equilibrium grades of ≥30% peroxyacetic acid exhibit both open and closed-cup flash points and are flammable.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for peroxyacetic acid.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Peroxyacetic acid will rapidly hydrolyse in water at high pH values (e.g., pH 9). It is readily biodegradable and is not expected to bioaccumulate. It has low potential to adsorb to sediment and soil.

B. Abiotic Degradation

Hydrolysis

In a hydrolysis test (EU Method C.7), the degradation half-lives of peroxyacetic acid at 25°C were 48, 48 and 3.6 hours at pH values of 4, 7 and 9. These results indicate that peroxyacetic acid is rapidly degraded in the environment and that decomposition is faster at high pH values (ECHA). [Kl. score = 2]

C. Biodegradation

Peroxyacetic acid was readily biodegradable in an OECD 301E test. The test material was applied gradually over a two-week period because addition of the full amount on day 0 caused inhibition of the microorganisms. After 14 days, DOC and TOC removal were 78% and 58%, respectively. After 28 days, DOC and TOC removal were 98% and 75%, respectively (ECHA). [Kl. score = 1]

Peroxyacetic acid tested in an OECD 209 test. Degradation was rapid, and the half-life was <3 minutes (ECHA). [Kl. score = 2]

D. Environmental Distribution

Adsorption/desorption

No experimental data are available for peroxyacetic acid. Using KOCWIN in EPISuite™ (USEPA, 2018), the estimated K_{oc} value from log K_{ow} is 1.27 L/kg. The estimated K_{oc} value from the molecular connectivity index (MCI) is 1.508 L/kg.

E. Bioaccumulation

There are no bioaccumulation studies on peroxyacetic acid. Peroxyacetic acid is not expected to bioaccumulate based on a log K_{ow} of -0.59 (ECHA).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Peroxyacetic acid has high acute toxicity by the oral and inhalation routes and moderate toxicity by the dermal routes. Depending on the concentration, aqueous solutions of peroxyacetic acid are either corrosive, irritating or non-irritating to the skin, eyes and gastrointestinal tract. Vapours from aqueous solutions of peroxyacetic acid can cause respiratory irritation. It is not a skin sensitiser. Repeated oral doses of peroxyacetic acid to rats showed no systemic toxicity. Peroxyacetic acid is not genotoxic. Developmental effects (but no teratogenicity) were seen in laboratory animals at oral doses that also were toxicity to the pregnant females.

B. Toxicokinetics

Following dermal application of radiolabelled peroxyacetic acid, absorption was rapid after an initial lag time of approximately one hour. Only a small portion of the administered dose (1%) was recovered as unchanged peroxyacetic acid, with 58% (as the mean) of the dose recovered as CO_2. The excretion via the faeces accounted for 3-4% of the administered radioactivity, tissue-bound radioactivity was 20% (as the mean) of the radioactivity, and urinary excretion was 11% (as the mean) of the radioactivity. The tissue-bound fraction likely represents the incorporation of formed acetic acid into the C2 pool involved in the metabolic pathways of the body (ECHA) [Kl. score = 2].

The half-life of peroxyacetic acid in rat blood is <5 minutes (ECHA). [Kl. score = 2]

C. Acute Toxicity

The acute oral LD_{50} values for peroxyacetic acid in the rat are shown in Table 3.

Table 3 Acute Oral LD_{50} Values of Peroxyacetic Acid in Rats

Test material (peroxyacetic acid concentration)	LD_{50} as test material (mg/kg)	LD_{50} as Peroxyacetic acid (mg/kg)	Klimisch score	Reference
0.15% solution	>5,000	>17.8	1	ECHA
0.89% solution	>2,000	>7.5	1	ECHA
2.6% solution	1,656	43	1	ECHA
5% solution	1,700-1,900 (m) 1,400 (f)	77-86 (m) 63 (f)	1	ECHA
4.89% solution	-	185	1	ECHA
5% solution	1,992	96.1	1	ECHA
5.6% solution	3,622	202.8	1	ECHA
6.1% solution	1,270	77.6	1	ECHA
10% solution	2,540 (m) 2,390 (f)	254 (m) 239 (f)	2	ECHA
11.7% solution	652	76.2	1	ECHA

Test material (peroxyacetic acid concentration)	LD_{50} as test material (mg/kg)	LD_{50} as Peroxyacetic acid (mg/kg)	Klimisch score	Reference
15% solution	1,026 (m) 1,015 (f)	153.9 (m) 152.3 (f)	2	ECHA
10% solution	1,780	271	1	ECHA

f = female
m = male

The 4-hour LC_{50} value of an aerosol of a 5% solution of peroxyacetic acid in rats is 204 mg/m^3 (ECHA) [Kl. score = 2].

The dermal LD_{50} of a 0.89% solution of peroxyacetic acid in rats is >2,000 mg/kg (>17.8 mg a.i./kg) (ECHA) [Kl. score = 1]. The dermal LD_{50} of a 4.89% solution of peroxyacetic acid in rats is 1,040 mg/kg (56.1 mg a.i./kg) (ECHA) [Kl. score = 1]. The dermal LD_{50} of a 11.7% solution of peroxyacetic acid in rats is 1,957 mg/kg (228.8 mg a.i./kg) (ECHA) [Kl. score = 1].

D. Irritation

Application of 0.5 mL of formulations containing 5%, 15% or 40% peroxyacetic acid to the skin of rabbits for 4 hours under occlusive conditions was corrosive (ECHA) [Kl. score = 1]. Application of 0.5 mL of formulations containing 0.034%, 0.34% or 3.4% peroxyacetic acid to the skin of rabbits for 24 hours under occlusive conditions were non-irritating, slightly irritating, and corrosive, respectively (ECHA) [Kl. score = 1]. Application of 0.5 mL of a formulation containing 5% peroxyacetic acid under occlusive conditions was moderately irritating after 3 minutes and corrosive after 45 minutes (ECHA) [Kl. score = 1]. Application of 0.5 mL of a formulation containing 15% peroxyacetic acid to the skin of rabbits for 4 hours under occlusive conditions was corrosive (ECHA) [Kl. score = 1].

Instillation of 0.1 mL of a formulation containing 0.15% peroxyacetic acid to the eyes of rabbits was corrosive (ECHA) [Kl. score = 1]. Instillation of 0.1 mL of a formulation containing 17% peroxyacetic acid to the eyes of rabbits was slightly irritating (ECHA) [Kl. score = 1].

E. Sensitisation

Peroxyacetic acid was not a skin sensitiser when tested on guinea pigs using the Magnusson-Kligman or Buehler methods (ECHA) [Kl. score = 1].

F. Repeated Dose Toxicity

<u>Oral</u>

Male and female SD rats were dosed by oral gavage with 0, 15, 50 or 150 mg/kg of a 5% peroxyacetic acid formulation from day 1 to 10 of the study; 0, 15, 50 or 100 mg/kg on days 11 to 22 of the study; and then 0, 5, 15 or 50 mg/kg on days 23 to 92 of the study. The doses on a time-weighted average were 0, 7.4, 23.4 and 67.4 mg/kg-day. No systemic effects were observed. In the high-dose group, 3/10 males and 9/10 females died or were killed prematurely between study days 8 and 71. In most of these animals symptoms of loud breathing, dyspnea, abdominal swelling or ptyalism were observed. Some of the surviving high-dose animals also showed ptyalism, loud breathing and/or

piloerection. One mid-dose female died showing reddened lungs with foamy content, lung congestion and alveolar oedema (this may indicate a death due to gavage error). Body weights and body weight gain in the high-dose animals were reduced compared to the controls. There were no treatment-related effects on hematology parameters, clinical chemistry or histopathology in the surviving animals in the high-dose or at the lower doses. In the high-dose animals that died or were killed prematurely, the stomach and several parts of the gastrointestinal tract were distended with gas and were reddish in colour; and the lungs were dilated. Treatment-related effects were also seen in the trachea (narcotizing inflammation) and lung (acute bronchitis at the tracheobronchial bifurcation) of these animals. Although the trachea and lungs were not directly in contact with the test material when administered by gavage, it is possible that rapid degradation of hydrogen peroxide and peroxyacetic acid occurred in the stomach and intestinal tract, resulting in release of oxygen gas that refluxed with the acidic stomach fluid into the trachea and lungs; this led to local irritation and an inflammatory response. The local effect NOAEL for this study is 23.4 mg/kg-day (ECHA). [Kl. score = 2]

Inhalation

No adequate studies are available.

Dermal

No adequate studies are available.

G. Genotoxicity

The results of the *in vitro* genotoxicity studies on solutions of peroxyacetic acid are shown in Table 4.

In Vitro Studies

Table 4 *In Vitro* Genotoxicity Studies on Peroxyacetic Acid Solutions

Test System	Results*		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* strains)[1]	-	-	1	ECHA
Bacterial reverse mutation (*S. typhimurium* strains)[2]	-	-	2	ECHA
Chromosomal aberration (Chinese hamster lung fibroblasts [V79])[3]	-	-	1	ECHA
Chromosomal aberration (human lymphocytes)[4]	+	+	2	ECHA
Unscheduled DNA synthesis (human lung fibroblasts [WI-38 CCL75])[5]	-	NA	2	ECHA

*+, positive; -, negative; NA, not applicable.
[1]4.6%peroxyacetic acid, 29.4% hydrogen peroxide, 7.4% acetic acid.
[2]40% peroxyacetic acid.
[3]10.7% peroxyacetic acid
[4]5.17% peroxyacetic acid, 20% hydrogen peroxide, 10% acetic acid.
[5]No composition information given.
NA = not applicable

In Vivo Studies

Male and female CF1/W 68 mice were given two oral gavage doses (24 hours apart) with 0, 200, 400 or 800 mg/kg of a formulation containing peroxyacetic acid. The concentrations of peroxyacetic acid were 0, 18, 36 and 72 mg/kg. There were no increases in the frequency of micronucleated erythrocytes in the bone marrow of treated mice compared to the controls (ECHA). [Kl. score = 2]

Male and female CD-1 mice were given a single oral gavage dose of 0, 8, 35 or 150 mg/kg of a formulation containing peroxyacetic acid. The concentrations of peroxyacetic acid were 0, 0.41, 1.8 and 7.8 mg/kg. There were no increases in the frequency of micronucleated erythrocytes in the bone marrow of treated mice compared to the controls (ECHA). [Kl. score = 1]

In an unscheduled DNA synthesis test, male F344 rats were given a single oral dose of 0, 1,000 or 2,000 mg/kg of a formulation containing peroxyacetic acid. The concentrations of peroxyacetic acid were 0, 52 and 104 mg/kg. There was no indication of a proliferative effect in the liver cells of the treated rats compared to the controls (ECHA). [Kl. score = 1]

In an unscheduled DNA synthesis test, male F344/DuCrj rats were given a single oral dose of 0, 330 or 1,000 mg/kg of a formulation containing peroxyacetic acid. The concentrations of peroxyacetic acid were 0, 17 and 52 mg/kg. There was no indication of a proliferative effect in the liver cells of the treated rats compared to the controls (ECHA). [Kl. score = 1]

H. Carcinogenicity

No studies are available.

I. Reproductive Toxicity

No adequate studies are available.

J. Developmental Toxicity

Pregnant female Wistar rats were given in their drinking water a test material containing 32-38% w/w peroxyacetic acid and 10-14% w/w hydrogen peroxide on GD 5-20. The doses were 0, 12.5, 30.4 and 48.1 mg peroxyacetic acid/kg-day and 0, 4.2, 10.1 and 16 mg hydrogen peroxide/kg-day. There were no maternal treatment-related clinical signs of toxicity or deaths. Food and water consumption were significantly reduced in the high-dose dams throughout the treatment period. The high-dose dams also had significantly reduced terminal body weights, corrected body weight and body weight gain from GD 5-20. Body weight gain in the lower dose females was transient and not significantly different from the controls by the end of the study. There was significantly reduced foetal body weights in the high-dose group and increased incidence of poor and/or hypertrophic ossification. The latter effect was thought to be a secondary effect to maternal toxicity. The effect on foetal weight in this dose group is also questionably treatment-related because the litter size was about 13% higher than in the controls which might have contributed to slightly smaller foetuses in this dose group. The most prominent finding in the study was a dose-dependent discoloration (greyish brown, yellowish or yellow) of the foetal livers, with the severity ranging from 5 to 100% when the size of discoloration or the affected area was taken into account. The incidence and severity of foetal liver discoloration was reported to increase with dose. Furthermore, a dose-related increase in the severity of foetal liver damage was observed and characterised by loosening or unrecognisable structure of liver parenchyma, degeneration to necrosis of the nuclei, atypical mitosis, lysis of hepatic cells, partly large blood islands with cell detritus and pyknotic nuclei. The foetal liver preparations were re-examined by an independent experienced veterinary pathologist and the laboratory pathologist responsible for this study. It was determined that the discoloration was a typical alteration of improperly chemically-fixed organs. Such discoloration is known to progress with time (wet tissue storage). The exact cause of the discoloration is unknown but may have been a consequence of the fixation method used. Thus, it was concluded that there was no treatment-related liver discoloration in the foetal liver and no foetal liver damage. The NOAEL for maternal and developmental toxicity was considered to be 30.4 mg a.i./kg-day (ECHA). [Kl. score = 2]

K. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for peroxyacetic acid follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

A 90-day oral gavage study was conducted on a 5% peroxyacetic acid formulation using rats. There was significant mortality, clinical signs, reduction in body weight and body weight gain. In the animals that died or were killed prematurely, histopathologic effects indicative of localised irritation and inflammation were seen in the gastrointestinal and respiratory tract. The NOAEL for this study is 23.4 mg a.i./kg-day. This NOAEL will be used for determining the oral Reference dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 3
UF_D (database uncertainty) = 1

Oral RfD = 23.4/(10 x 10 x 1 x 3 x 1) = 23.4/300 = 0.08 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.08 x 70 x 0.1)/2 = 0.3 mg/L

Cancer

There are no carcinogenicity studies on peroxyacetic acid. Thus, a cancer reference value was not derived.

L. Human Health Hazard Assessment of Physico-Chemical Properties

Peroxyacetic acid is classified as a Category 3 Flammable Liquid.

Peroxyacetic acid does not exhibit the following physico-chemical properties:

- Explosivity
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Peroxyacetic acid is highly toxic to aquatic organisms on both an acute and chronic basis.

B. Aquatic Toxicity

Acute Studies

Table 5 lists the results of the acute aquatic toxicity studies on peroxyacetic acid.

Table 5 Acute Aquatic Toxicity Studies on Peroxyacetic Acid

Test Species	Endpoint	Results (mg a.i./L)	Klimisch score	Reference
Oncorhynchus mykiss	96-h LC_{50}	0.53	2	ECHA
Lepomis macrochirus	96-h LC_{50}	1.1	2	ECHA
Oncorhynchus mykiss	96-h LC_{50}	1.0	2	ECHA
Lepomis macrochirus	96-h LC_{50}	1.2	2	ECHA
Oncorhynchus mykiss	96-h LC_{50}	2.0	2	ECHA
Danio rerio	96-h LC_{50}	1.1	2	ECHA
Oncorhynchus mykiss	96-h LC_{50}	0.08 (measured)	1	ECHA
Danio rerio	96-h LC_{50}	1.0	2	ECHA
Daphnia magna	48-h EC_{50}	0.73	2	ECHA
Daphnia	48-h LC_{50}	1.1	2	ECHA
Daphnia magna	48-h EC_{50}	1.94	2	ECHA
Daphnia magna	48-h EC_{50}	0.5	2	ECHA
Daphnia	48-h EC_{50}	0.48	2	ECHA
Pseudokirchneriella subcapitata	72-h EC_{50} NOEC	0.16 0.061	1	ECHA
Pseudokirchneriella subcapitata	72-h EC_{50} NOEC	0.86 0.084	1	ECHA
Desmodesmus subspicatus	72-h EC_{50} NOEC	1.6 0.27	2	ECHA

Chronic Studies

The NOEC from a 33-day fish (*Danio rerio*) early-life stage toxicity test was 0.002 mg a.i./L (ECHA). [Kl. score = 2]

The NOEC from a *Daphnia* reproduction test was 0.012 mg a.i./L (ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

Earthworms

In an OECD TG 207 test, the 14-day LC_{50} value for peroxyacetic acid in the earthworm *Eisenia fetida* was >1,000 mg a.i./kg soil dry weight (ECHA). [Kl. score = 1]

Terrestrial Plants

Peroxyacetic acid has also been evaluated in a seedling emergence and seedling growth (OECD TG 208) test (ECHA) [Kl. score = 1]. The results (expressed as active ingredient) are presented in Table 6.

Table 6 Terrestrial Plant Toxicity Test (OECD 208) Results* on Peroxyacetic Acid

Plant	21-day EC_{25}	21-day EC_{50}	21-day NOEC
Brassica napus	278	>320	180
Glycine max (*G. soja*)	307	328	180
Avena sativa	363	413	180

*mg/kg soil dry weight based on seedling emergence.

Soil Organisms

In the soil microorganisms nitrogen transformation (OECD TG 216) test, the EC_{25} and the EC_{50} values for peroxyacetic acid were 813 and >933.3 mg a.i./kg soil dry weight, respectively. The 28-day NOEC was 295.2 mg a.i./kg soil dry weight (ECHA). [Kl. score = 1]

D. Calculation of PNEC

The PNEC calculations for peroxyacetic acid follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (0.08 mg/L), invertebrates (0.48 mg/L), and plants (0.16 mg/L). Results from chronic studies are also available for all three trophic levels, with the lowest NOEC being 0.002 mg/L for fish. On the basis that the data consist of short-term and long-term results from three trophic levels, an assessment factor of 10 has been applied to the lowest reported NOEC of 0.002 mg/L for fish. The $PNEC_{water}$ is 0.0002 mg/L or 2×10^{-4} µg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.00013 mg/kg wet weight or 1.3×10^{-4} µg/kg wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (0.824/1280) \times 1000 \times 0.0002$
$= 0.00013$

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times (Kp_{sed}/1000) \times BD_{soilid}]$
$= 0.8 + [0.2 \times (0.05/1000) \times 2400]$
$= 0.824$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 1.27 \times 0.04$
$= 0.05$

Where:

K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for peroxyacetic acid based on log K_{ow} is 1.27 L/kg.
F_{oc} = fraction of organic carbon suspended sediment = 0.04 [default]

PNEC soil

Experimental results are available for three trophic levels. An acute LC_{50} value is available for earthworms (>1,000 mg/kg soil dry weight). Results from long-term studies are available for two trophic levels, with the lowest NOEC being 180 mg/kg soil dry weight for all three plant species. On the basis that the data consist of short-term and long-term tests from two trophic levels, an assessment factor of 50 has been applied to the lowest reported long-term NOEC of 180 mg/kg soil dry weight. The $PNEC_{soil}$ is 3.6 mg/kg soil dry weight.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Peroxyacetic acid is readily biodegradable. Thus, it does not meet the screening criteria for persistence.

The experimental log K_{ow} for peroxyacetic acid is -0.59. Thus, it does not meet the screening criteria for bioaccumulation.

The lowest NOEC from chronic aquatic toxicity studies on peroxyacetic acid is <0.1 mg/L. Thus, it meets the criteria for toxicity.

The overall conclusion is that peroxyacetic acid is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, peroxyacetic acid does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for peroxyacetic acid.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Peroxyacetic Acid	79-21-0	Not a PBT	No	No	No	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
a.i.	active ingredient
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre

GD	gestation day
HHRA	enHealth Human Risk Assessment
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metres
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilo pascal
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SD	Sprague Dawley
SGG	Synthetic Greenhouse Gases
TG	Test Guideline
TOC	total organic carbon
USEPA	United States Environmental Protection Agency

Qualitative and Quantitative Tier 3 Assessment

Sodium Hypochlorite

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Sodium hypochlorite is a component in a Water Management Facility (WMF) product used as an oxidising agent/disinfectant during oily water treatment. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals – Tier 3 Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
Sodium Hypochlorite Sodium Hydroxide	7681-52-9 1310-73-2	Oxidising agent/disinfectant	15000 L

CAS No = Chemical Abstracts Service Number
L = litre

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. Since an Australian Drinking Water Guideline (ADWG) Value is available (see **Table 2**), toxicological reference values (TRVs) were not derived for the chemical. A detailed discussion of the drinking water guideline values is presented in **Attachment 2**.

Table 2 Australian Drinking Water Screening Values

Constituent (CAS No.)	Drinking Water Screening Guideline	Drinking Water Screening Value
Sodium hypochlorite (7681-52-9)	Chlorine	5 mg/L (health) and 0.6 mg/L (aesthetics)

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of TRVs was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effect concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). A PNEC for soil was not calculated for the chemical. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Sodium hypochlorite (7681-52-9)	-	-	-	0.003[a]

[a] $PNEC_{water}$ for sodium hypochlorite is the Australian and New Zealand Guidelines (ANZG) Water Quality Guideline – Freshwater Trigger Value for chlorine.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

Sodium hypochlorite is a yellow, limpid liquid with a chlorinated odour. The molecular structure of sodium hypochlorite is presented in **Figure 1**.

Figure 1 Molecular Structure of Sodium Hypochlorite[2]

In water, sodium hypochlorite (NaClO) dissociates into the sodium (Na^+) ion and the hypochlorite (ClO^-) ion. The hypochlorite ion (ClO^-) is in equilibrium with hydrochlorous acid (HClO) in water and chlorine gas (Cl_2), with the relative amounts determined by pH, temperature and ionic strength of the water. Free chlorine (Cl_2) reacts with ammonia and certain nitrogen compounds to form N-chlorinated compounds. These compounds are more persistent than the free chlorine. N-chloramines are intentionally produced in water treatment to extend the effectiveness of chlorination.

Biodegradation is not applicable to sodium hypochlorite. Sunlight (ultraviolet light) will rapidly decompose sodium hypochlorite to sodium chloride (OxyChem, 2014). Sodium hypochlorite and its dissociated ions are ubiquitous in the environment. They are not expected to adsorb to soil or sediment and are not bioaccumulative.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for sodium hypochlorite is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that sodium hypochlorite is not a PBT substance.

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/7681-52-9

Human Health Hazards

Sodium hypochlorite solutions have low acute toxicity by the oral and dermal routes. It is corrosive to the skin, eyes and the gastrointestinal tract. Based on human and animal data, sodium hypochlorite concentrations over 5% are irritating to the skin and eye, while concentrations over 10% are corrosive. Aerosolised sodium hypochlorite is a respiratory irritant. It is not a skin sensitiser (NICNAS, 2017).

No systemic, reproductive or developmental toxicity was seen in rats in repeated dose toxicity and reproductive/developmental toxicity studies. While sodium hypochlorite has been positive in some *in vitro* genotoxicity studies, the *in vivo* studies have been negative. Sodium hypochlorite was not carcinogenic to rats or mice in chronic drinking water studies.

Toxicological reference values were not derived for sodium hypochlorite. The ADWG values for chlorine are 5 mg/L (health) and 0.6 mg/L (aesthetics).

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the treatment process described in **Attachment 1**, sodium hypochlorite fully dissociates to sodium (Na) and chloride (Cl), with Na and Cl removed by the reverse osmosis (RO) system at 95% to the brine and 5% stays within permeate. Sodium concentrations are *de minimis* (< 10 mg/L) in the permeate and <80 mg/L in the brine, both of which are less than geogenic background. As a result, this chemical was not evaluated further in the permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

Sodium hypochlorite is very toxic to aquatic organisms. Sodium hypochlorite (NaClO) dissociates into the sodium (Na^+) ion and the hypochlorite (ClO^-) ion in aqueous media. As an inorganic salt, neither sodium hypochlorite nor its dissociated ions are expected to bioaccumulate. The acute and subacute oral toxicity of sodium hypochlorite to birds are of low concern.

In standard aquatic toxicity tests, sodium hypochlorite is highly toxic to aquatic organisms on both an acute and chronic basis. In the acute aquatic tests, algae were found to be the most sensitive species. Fish and *daphnia* were less susceptible. Acute terrestrial toxicity tests are available for

earthworm, plants and soil microorganisms. Under typical environmental conditions, the chemical is expected to degrade rapidly in soil and water and does not persist in the environment. The chemical also does not bioaccumulate.

The water quality guideline (ANZG, 2018) used acute and chronic laboratory toxicity data for the derivation of a trigger value for chlorine. The guideline for freshwater is: "A freshwater moderate trigger value of 3 µg Cl/L measured as total residual chlorine was derived using the statistical distribution method with 95% protection. This figure was obtained from the application of the default ACR of 10 instead of the empirical ACR of 2.7 from the geometric mean of 8 figures. The smaller ACR would have resulted in a value not protective of some species under continuous exposure to chlorine for at least 48 hours". Considering the land uses adjacent to the Dawson River include light to moderate grazing, and there is some development upstream of the Horseshoe Lakes, adoption of the 95% species protection criteria is considered appropriate (AECOM, 2019).

No experimental toxicity data on sediment or soil organisms are available. Octanol/water partition coefficient (K_{ow}) and organic carbon-water partition coefficient (K_{oc}) parameters do not readily apply to inorganics, such as sodium hypochlorite. Thus, the equilibrium partitioning method cannot be used to calculate PNECs for soil or sediment. Based on its properties, sodium hypochlorite is not expected to significantly adsorb to soil or sediment, and the assessment of these compartments is covered by the aquatic assessment.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River. AECOM (2016) in their assessment concluded that stock watering occurred well outside the 1.4 km mixing zone within the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to sodium hypochlorite that may occur during water treatment activities. The risk characterisation evaluates the toxicity of sodium hypochlorite and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, sodium hypochlorite would not be present in permeate, brine or treated water above geogenic background levels. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), sodium hypochlorite does not meet the criteria for persistence or bioaccumulation. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in

environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 4** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 4 Evaluation of Uncertainty – Sodium Hypochlorite

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in the water treatment process were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Hazard Assessment –COPC concentrations	Concentrations of COPCs evaluated in the quantitative risk assessment were assumed to be 100 percent of mass used in the water treatment process. This is a conservative assumption for chemicals that may degrade rapidly or volatilise.	Medium	This assumption may overestimate the calculated risks to receptors.
Toxicity Assessment	The absence of terrestrial toxicity data and the lack of a Koc value to calculate a PNEC in soil or sediment.	Medium	Medium to high potential to underestimate risks.

References

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Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		On-site Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Sodium Hypochlorite Solution 12.5%	Sodium Hypochlorite	7681-52-9	10-30%	Hypochlorite Solution	Coogee Chemicals	Reverse Osmosis Plant	10000L	12.50%	15000L	12.50%	18-35L/hour (25 AVG)	12.50%	220000L	oxidizing agent / disinfectant
	Sodium Hydroxide	1310-73-2	<10%											

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concentration
L = litres
L/hr = litre per hour
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
RO = reverse osmosis
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration
				(mg/L)	Permeate notes	(mg/kg)	(mg/kg)	(mg/L)
Sodium Hypochlorite Solution 12.5%	Sodium Hypochlorite	7681-52-9	Converted to monochloramine and sodium metabisulphite dosing prior to RO membranes	NA	Fully dissociates to sodium (Na) and chloride (Cl) removed by the RO system (95%) goes to brine, 5% stays within permeate. Na concentrations are diminimis (< 10 mg/L), residual Na would be less than 4 mg/L. Na and Cl residual concentrations are consistent with or less than geogenic background.	NA	NA	NA
	Sodium Hydroxide	1310-73-2		NA	Fully dissociates to Na and hydroxyl ion (OH^-), with Na and OH^- removed by the RO system at 95% to the brine and 5% stays within permeate. Na concentrations are diminimis (< 10mg/L) and consistent with or less than geogenic background.	NA	NA	NA

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concentration
L = litres
L/hr = litre per hour
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
RO = reverse osmosis
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Brine Notes
Sodium Hypochlorite Solution 12.5%	Sodium Hypochlorite	7681-52-9	Fully dissociates with Na removed by the RO system (95%) will go to brine. Residual Na would be less than 80 mg/L in brine, which is consistent or less than geogenic background.
	Sodium Hydroxide	1310-73-2	Fully dissociates to Na and hydroxyl ion (OH-), with Na and OH- removed by the RO system at 95% to the brine dams. However, concentrations of Na consitient or less than geogenic background.

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concentration
L = litres
L/hr = litre per hour
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
RO = reverse osmosis
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

SODIUM HYPOCHLORITE

This dossier on sodium hypochlorite presents the most critical studies pertinent to the risk assessment of sodium hypochlorite in its use in water treatment systems. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sodium hypochlorite was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. Sodium hypochlorite was assessed as a tier 3 chemical for acute toxicity and as a tier 3 chemical for chronic toxicity. Therefore, sodium hypochlorite is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

Sodium hypochlorite is a yellow, limpid liquid with a chlorinated odour. In water, sodium hypochlorite (NaClO) dissociates into the sodium (Na^+) ion and the hypochlorite (ClO^-) ion. The hypochlorite ion (ClO^-) is in equilibrium with hydrochlorous acid (HClO) in water and chlorine gas (Cl_2) , with the relative amounts determined by pH, temperature and ionic strength of the water. Between pH 2 and 7, hydrochlorous acid (HClO) is the dominant form; at pH 7.4 and 20^{o}C, there is equimolar contribution of HClO and ClO-. Sodium hypochlorite (NaClO) dissociates into the sodium (Na^+) ion and the hypochlorite (ClO^-) ion in aqueous media. Biodegradation is not applicable to sodium hypochlorite. Sunlight (UV light) will rapidly decompose sodium hypochlorite to sodium chloride. Sodium hypochlorite and its dissociated ions are ubiquitous in the environment. They are not expected to adsorb to soil or sediment and are not bioaccumulative. Aqueous solutions of sodium hypochlorite can be irritating to corrosive to the skin, eyes and gastrointestinal tract, depending on the concentration. Inhalation of vapours for aqueous solutions of sodium hypochlorite can cause respiratory irritation. It is not a skin sensitiser. Lifetime studies have shown no toxicity or carcinogenic effects in rats and mice when given sodium hypochlorite in their drinking water. While sodium hypochlorite has been positive in some in vitro genotoxicity studies, the in vivo studies have been negative. Sodium hypochlorite is not a reproductive or developmental toxicant. Sodium hypochlorite is very toxic to aquatic organisms. The acute and subacute oral toxicity of sodium hypochlorite to birds are of low concern.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium hypochlorite

CAS RN: 7681-52-9

Molecular formula: NaClO

Molecular weight: 74.44

Synonyms: Sodium hypochlorite; hypochlorous acid, sodium salt; bleach; chlorine bleach

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Sodium Hypochlorite

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Yellow, limpid liquid with a chlorinated odour	1	ECHA
Melting Point	-28.9°C	1	ECHA
Boiling Point	>60.4°C (decomposition)	1	ECHA
Density	1.3 @ 21.2°C*	1	-
Vapour Pressure	ca. 2.5 kPa @ 20°C	2	ECHA
Partition Coefficient (log K_{ow})	Not applicable	-	-
Water Solubility	Very soluble	-	ECHA
Flash Point	>111°C @ 101.3 kPa	1	ECHA
Auto flammability	-	-	-
Oxidising properties	None	1	ECHA
pH (5% solution) pH (1% solution)	12.52 @ 19.1°C 10.30 @ 21.3°C	1	ECHA
Viscosity	1.4-1.6 mPa.s @ 20°C 1.4-1.6 mPa.s @ 40°C	1	ECHA

*Sodium hypochlorite with 24.3% available chlorine.

In water, sodium hypochlorite (NaClO) dissociates into the sodium (Na^+) ion and the hypochlorite (ClO^-) ion.

The hypochlorite ion (ClO^-) is in equilibrium with hydrochlorous acid (HClO) in water and chlorine gas (Cl_2), with the relative amounts determined by pH, temperature and ionic strength of the water. At very extremely low pH, chlorine gas (Cl_2) is essentially un-hydrolysed and is thus the dominant species of chlorine. Note that the term free chlorine refers to Cl_2. Between pH 2 and 7, hydrochlorous acid (HClO) is the dominant form; at pH 7.4 and 20°C, there is the equimolar contribution of HClO and ClO^-.

The chemical reactions are as follows:

$Cl_2 + H_2O \rightleftharpoons HClO + HCl$

$HClO \rightleftharpoons ClO^- + H^+$

Free chlorine reacts with ammonia and certain nitrogen compounds to form N-chlorinated compounds. With ammonia, chlorine forms chloramines (monochloramine, dichloramine, and nitrogen chloride or trichloramine. These compounds constitute what is termed combined chlorine. These compounds are more persistent than the free chlorine. Monochloramine contributes significantly to the combined available chlorine in the water. N-chloramines are intentionally produced in water treatment to extend the effectiveness of chlorination.

Free chlorine and combined chlorine may be present simultaneously in a water sample. The term total chlorine or total residual chlorine (TRC) refers to the sum of free chlorine and combined chlorine that is present in a water sample.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium hypochlorite.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

Sodium hypochlorite (NaClO) dissociates into the sodium (Na^+) ion and the hypochlorite (ClO^-) ion in aqueous media. Biodegradation is not applicable to sodium hypochlorite. Sunlight (UV light) will rapidly decompose sodium hypochlorite to sodium chloride (OxyChem, 2014). Sodium hypochlorite and its dissociated ions are ubiquitous in the environment. They are not expected to adsorb to soil or sediment and are not bioaccumulative.

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

Aqueous solutions of sodium hypochlorite can be irritating to corrosive to the skin, eyes and gastrointestinal tract, depending on the concentration. Inhalation of vapours for aqueous solutions of sodium hypochlorite can cause respiratory irritation. It is not a skin sensitiser. Lifetime studies have shown no toxicity or carcinogenic effects in rats and mice when given sodium hypochlorite in their drinking water. While sodium hypochlorite has been positive in some *in vitro* genotoxicity studies, the *in vivo* studies have been negative. Sodium hypochlorite is not a reproductive or developmental toxicant.

B. Acute Toxicity

The oral LD_{50} of a sodium hypochlorite solution (12.2% active chlorine) in rats was 8,830 mg/kg, which was calculated to be 1,100 mg/kg based on average Cl_2 (ECHA) [Kl. score = 2]. The oral LD_{50} of

undiluted sodium hypochlorite in rats was 8,910 mg/kg (ECHA) [Kl. score = 2]. The oral LD_{50} of sodium hypochlorite (given as a12.5% solution) was 5,230 mg/kg.

The dermal LD_{50} in rabbits is >20,000 mg/kg (ECHA). [Kl. score = 2]

The 1-hour LC_{50} in rats is >10.5 mg/L (ECHA). [Kl. score = 2]

C. Irritation

A 12.5% solution of sodium hypochloride was irritating to the skin of rabbits when 0.5 ml was applied for 24 hours under semi-occlusive conditions. The mean of the 24 and 72 hours scores were: 2.16 for erythema and 1.04 for edema (ECHA) [Kl. score = 2]. Application of 0.1 mL of sodium hypochlorite (5.25% solution) to the intact skin of rabbits for 24 hours under semi-occlusive conditions was slightly irritating but not sufficient for classification as an irritant. The 24 and 72-hour mean scores were: 1.17 for erythema and 0.13 for edema (ECHA) [Kl. score = 2]. In another study, application of sodium hypochlorite (5.25% solution) to the intact skin of rabbits and guinea pigs was slightly irritating (ECHA) [Kl. score = 2].

Instillation of 0.1 g of sodium hypochlorite into the eyes of rabbits was irritating without full recovery after 7 days (ECHA) [Kl. score = 2].

D. Sensitisation

Sodium hypochlorite was not a skin sensitiser in guinea pig maximisation tests (ECHA). [Kl. score = 2]

E. Repeated Dose Toxicity

Oral

Male and female F344/N rats were given in their drinking water 0, 0.025%, 0.05%, 0.1%, 0.2%, and 0.4% sodium hypochlorite solution for 90 days. The concentrations correspond to daily intakes of: 0, 12.5, 25, 50, 100 and 200 mg/kg-day for males and 14.3, 28.6, 57.2, 114.4 and 228.8 mg/kg-day for females, assuming a daily water consumption of 25 mL and mean body weights of 0.5 kg for males and 0.35 kg for females. There were deaths during the study. Body weight gain was significantly reduced in the ≥0.2% males and 0.4% females. There were no treatment-related changes noted at necropsy, although several animals, particularly in the 0.4% group, appeared emaciated. Absolute weights of the lung, liver and spleen of males and the salivary gland, lung, heart and brain of females were significantly lower in the 0.4% groups compared to controls. Biochemical changes in the ≥0.2% groups indicated possible liver toxicity, but there were no corresponding histopathological changes in the liver; nor was there any other treatment-related histopathological changes. The NOAEL for this study is 0.1% in drinking water (50 and 57 mg/kg-day for males and females, respectively) (Hasewaga et al., 1986; ECHA). [Kl. score = 1]

Male and female F344/N rats were given sodium hypochlorite in their drinking water for 103-104 weeks. The concentrations were 0, 500 and 1000 ppm for males and 0, 1,000 and 2,000 ppm for females. The corresponding doses were estimated to be: 0, 25 and 50 mg/kg-day for males; and 0, 57 and 114 mg/kg-day for females (assuming body weights of 0.5 mg for males and 0.35 mg for females and a daily water intake of 25 mL). Survival was similar across all groups. Body weight gain was reduced in both male and female rats. Water consumption was comparable among all groups.

No significant dose-related changes in haematology and clinical chemistry. In rats, the incidences of non-neoplastic lesions (chronic nephropathy in treated males, granulomatous changes in the liver of treated females) were significantly decreased. The NOAELs are 50 and 114 mg/kg-day for males and females, respectively (Kurokawa et al. 1986; Hasegawa et al., 1986; ECHA).

Male and female B6C3F1 mice were given sodium hypochlorite in their drinking water for 103-104 weeks. The concentrations were 0, 500 and 1000 ppm (corresponding to 83.3 and 166.7 mg/kg-day for males; and 100 and 200 mg/kg-day for females). Survival was similar across all groups. Body weight gain was reduced in both male and female rats. Water consumption was comparable among all groups. No significant dose-related changes in haematology and clinical chemistry. In rats, the incidences of non-neoplastic lesions (chronic nephropathy in treated males, granulomatous changes in the liver of treated females) were significantly decreased. The NOAELs are 167 and 200 mg/kg-day for males and females (Kurokawa et al., 1986; ECHA).

Male and female F344/N rats were given sodium hypochlorite in their drinking water for 104 weeks. The concentrations were 0, 70, 140 and 275 ppm (corresponding to 0, 3.5, 7 and 13.75 mg/kg-day for males and 0, 4, 8 and 15.7 mg/kg-day for females assuming a body weight of 0.5 and 0.35 g and a water consumption of 25 mL/day). Palatability was the principal factor limiting the concentrations of available chlorine in the study. There was a dose-related decrease in water consumption by animals receiving chlorinated water. Decreased water consumption was evident during the first week and continued throughout the study. Toward the end of the studies, the effect on water consumption was less than during the first weeks. The animals showed no physiological alterations due to decreased water consumption, and there was no clinical or haematological evidence of dehydration. Because body weight and water consumption changed as the rats aged, the amount of available chlorine ingested during the study varied. The mean daily dose (mg/kg body weight) was higher during the first 13 weeks than during the second year of the studies. High-dose rats received a mean daily dose of approximately 20 mg/kg for the first 13 weeks, which decreased to 13-14 mg/kg during the second year. Survival of rats was similar among treated groups and their respective controls. Survival of all groups of male rats was less than 50% at the end of the studies. There were no treatment-related lesions in rats at the 14-week or at the 66-week interim evaluations. There were no non-neoplastic lesions that were clearly attributable to the consumption of chlorinated water. The applied chlorine concentrations were well tolerated; there were no treatment-related clinical signs, mortalities, haematological or histopathological findings. The NO(A)EL > 275 ppm (13.75 mg/kg-day for males and 15.7 mg/kg-day for females) (NTP, 1992).

Male and female B6C3F_1 mice were given sodium hypochlorite in their drinking water for 104 weeks. The concentrations were 0, 70, 140 and 275 ppm (corresponding to 0, 11.7, 23.3 and 45.8 mg/kg-day for males and 0, 14, 28 and 55 mg/kg-day for females assuming a body weight of 300 kg and 250 kg and a water consumption of 5 mL/day). Palatability was the principal factor limiting the concentrations of available chlorine in the study. There was a dose-related decrease in water consumption by animals receiving chlorinated water. Decreased water consumption was evident during the first week and continued throughout the study. Toward the end of the studies, the effect on water consumption was less than during the first weeks. The animals showed no physiological alterations due to decreased water consumption, and there was no clinical or haematological evidence of dehydration. Because body weight and water consumption changed as the mice aged, the amount of available chlorine ingested during the study varied. The mean daily dose (mg/kg body weight) was higher during the first 13 weeks than during the second year of the studies. High-dose mice received a mean daily dose of approximately 35-44 mg/kg for the first 13 weeks, which decreased to 20-23 mg/kg during the second year. Survival was similar among treated groups and

their respective controls. There were no treatment-related lesions in mice at the 15-week or at the 66-week interim evaluations. There were no non-neoplastic lesions that were clearly attributable to the consumption of chlorinated water. The applied chlorine concentrations were well tolerated; there were no treatment-related clinical signs, mortalities, haematological or histopathological findings. The NOAEL was >275 ppm (45.8 mg/kg-day for males and 55 mg/kg-day for females) (NTP, 1992).

Inhalation

No studies were located.

Dermal

No studies were located.

F. Genotoxicity

In Vitro Studies

The *in vitro* genotoxicity studies on sodium hypochlorite are summarised in Table 3.

Table 3 In Vitro Genotoxicity Studies on Sodium Hypochlorite

Test System	Results[a]		Klimisch Score	Reference
	-S9	+S9		
Bacterial reverse mutation (*S. typhimurium* TA98, TA100)	-	+ (TA100 only)	2	ECHA
Bacterial reverse mutation (*S. typhimurium* TA98, TA100, TA102)	-	NC	1	ECHA
Bacterial reverse mutation (*S. typhimurium* TA98, TA100, TA1535, TA1537	-	+ (TA100 only)	1	ECHA
Chromosomal aberration (Chinese Hamster Lung cells)	[b]	+	2	ECHA
Chromosomal aberration (human HE2144 fibroblasts)	Ambiguous	NC	2	ECHA
E. coli PQ37 – SOS Chromotest [DNA repair]	-	-	2	ECHA
S. cerevisiae gene mutation assay	+	-	2	ECHA
Comet assay (human lymphocytes)	+	NC	2	ECHA

[a]+, positive; -, negative; NC, not conducted.
[b]No results since all concentrations were cytotoxic.
TA100 = Salmonella typhimurium strain TA100

In Vivo Studies

The *in vivo* studies on sodium hypochlorite are presented below in Table 4. Sodium hypochlorite was not mutagenic or genotoxic.

Table 4 *In Vivo* Genotoxicity Studies on Sodium Hypochlorite

Test System	Results*	Klimisch Score	Reference
Mouse bone marrow micronucleus (intraperitoneal, 1 or 4 consecutive days)	-	1	ECHA
Mouse bone marrow micronucleus (oral gavage, 1 or 5 consecutive days)	-	2	ECHA
Mouse bone marrow chromosomal aberration (oral gavage, 1 or 5 consecutive days	-	2	ECHA
Rat liver and kidney 8-hydroguanosine [DNA adduct] levels (oral, single dose)	-	2	ECHA
Mouse sperm head morphology	Ambiguous	2	ECHA

*+, positive; -, negative

G. Carcinogenicity

Oral

Male and female F344/N rats were given sodium hypochlorite in their drinking water for 103-104 weeks. The concentrations were 0, 500 and 1,000 ppm for males and 0, 1,000 and 2,000 ppm for females. The corresponding doses were estimated to be: 0, 25 and 50 mg/kg-day for males; and 0, 57 and 114 mg/kg-day for females (assuming body weights of 0.5 mg for males and 0.35 mg for females and a daily water intake of 25 mL). Survival was similar across all groups. Water consumption was comparable across all groups. There was no evidence of carcinogenicity in the treated animals (Kurokawa et al. 1986; Hasegawa et al., 1986; ECHA).

Male and female B6C3F1 mice were given sodium hypochlorite in their drinking water for 103-104 weeks. The concentrations were 0, 500 and 1,000 ppm (corresponding to 83.3 and 166.7 mg/kg-day for males; and 100 and 200 mg/kg-day for females). Survival was similar across all groups. Body weight gain was reduced in both male and female rats. Water consumption was comparable among all groups. There was no evidence of carcinogenicity in the treated mice (Kurokawa et al., 1986; ECHA).

Male and female F344/N rats were given sodium hypochlorite in their drinking water for 104 weeks. The concentrations were 0, 70, 140 and 275 ppm (corresponding to 0, 3.5, 7 and 13.75 mg/kg-day for males and 0, 4, 8 and 15.7 mg/kg-day for females assuming a body weight of 500 g for males and 350 g for females and a water consumption of 25 mL/day). Palatability was the principal factor limiting the concentrations of available chlorine in the study. There was a dose-related decrease in water consumption by animals receiving chlorinated water. Decreased water consumption was evident during the first week and continued throughout the study. Toward the end of the studies, the effect on water consumption was less than during the first weeks. The animals showed no physiological alterations due to decreased water consumption, and there was no clinical or haematological evidence of dehydration. Because body weight and water consumption changed as the rats aged, the amount of available chlorine ingested during the study varied. The mean daily dose (mg/kg body weight) was higher during the first 13 weeks than during the second year of the studies. High-dose rats received a mean daily dose of approximately 20 mg/kg for the first 13 weeks, which decreased to 13-14 mg/kg during the second year. Survival of rats was similar among treated groups and their respective controls. Survival of all groups of male rats was less than 50% at the end

of the studies. There were no neoplasms lesions that were clearly attributable to the consumption of chlorinated water. Under the conditions of this 2-year drinking water study, there was no evidence of carcinogenic activity of chlorinated water in F344/N rats receiving 70, 140 or 275 ppm (NTP, 1992).

Male and female B6C3F_1 mice were given sodium hypochlorite in their drinking water for 104 weeks. The concentrations were 0, 70, 140 and 275 ppm (corresponding to 0, 11.7, 23.3 and 45.8 mg/kg-day for males and 0, 14, 28 and 55 mg/kg-day for females assuming a body weight of 30 g for males and 25 g for females and a water consumption of 5 mL/day). Palatability was the principal factor limiting the concentrations of available chlorine in the study. There was a dose-related decrease in water consumption by animals receiving chlorinated water. Decreased water consumption was evident during the first week and continued throughout the study. Toward the end of the studies, the effect on water consumption was less than during the first weeks. The animals showed no physiological alterations due to decreased water consumption, and there was no clinical or haematological evidence of dehydration. Because body weight and water consumption changed as the mice aged, the amount of available chlorine ingested during the study varied. The mean daily dose (mg/kg body weight) was higher during the first 13 weeks than during the second year of the studies. High-dose mice received a mean daily dose of approximately 35-44 mg/kg for the first 13 weeks, which decreased to 20-23 mg/kg during the second year. Survival was similar among treated groups and their respective controls. There were no neoplasms lesions that were clearly attributable to the consumption of chlorinated water. Sporadically renal neoplasms occurred in the low and high-dose males. This is an unusual finding in mice. Therefore, additional step sections of the kidney were prepared which revealed further incidences of renal hyperplasia in all groups including control and a carcinoma in the low dose group. Nearly all the additional neoplasms seen in the step sections were small (microscopic) adenomas believed to be the probable precursor of renal tubule carcinoma. Since no additional renal neoplasms were found in the mid and high-dose groups and since focal hyperplasia, a potential pre-neoplastic lesion, was found at similar incidences in the control and dosed groups, the small number of renal tubule cell neoplasms in male mice were not considered related to the consumption of chlorinated water. Under the conditions of this 2-year drinking water study, there was no evidence of carcinogenic activity of chlorinated water in male or female B6C3F_1 mice receiving 70, 140 or 275 ppm (NTP, 1992).

H. Reproductive Toxicity

In a one-generation reproductive toxicity study, male and female Long-Evans rats were given in their drinking water 0, 1, 2 or 5 mg/kg-day dose of sodium hypochlorite. Males were dosed 56 days prior to and during mating. Females were dosed 14 days prior to mating, during mating, gestation and until lactation day 21. There were no adverse effects on reproduction or development, including histopathology of the reproductive organs in males and females, sperm parameters in males and histopathologic effects in the non-reproductive organs in females. The NOAEL for reproductive and developmental toxicity is 5 mg/kg-day (Carlton et al., 1986; ECHA). [Kl. score = 2]

I. Developmental Toxicity

Female SD rats were given in their drinking water 0, 1, 10 or 100 mg/L sodium hypochlorite for 2.5 months prior to mating and throughout gestation. Maternal toxicity was not examined. There were no treatment-related effects on viability, foetal weights, and external appearances of the foetuses in all dose groups. The foetuses of the $\geq$10 mg/L groups had a non-statistically significantly higher percentage of skeletal defects compared to controls. The 100 mg/L group also had a non-statistically

significantly higher rate of soft-tissue defects. These defects consisted of three cases of adrenal agenesis, one right-sided heart, one case of improper orientation of the apex of the heart, and one atrio-ventricular valve enlargement. The 100 mg/L group had a statistically significantly higher number of total defects; whereas the 1 mg/L dose had a lower percentage of defects compared to controls. In the absence of a clear dose-response and a relatively higher incidence of defects in the control animals, these findings were not considered to be of toxicological relevance. The NOAEL for developmental toxicity in this study was considered to be 100 mg/L, corresponding to 50 mg/kg-day (Abdel-Rahmen et al., 1982; ECHA). [Kl. score = 2]

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

Non-Cancer

An oral toxicological reference value was not derived for sodium hypochlorite.

The Australian drinking water guideline values for chlorine are 5 mg/L (health) and 0.6 mg/L (aesthetics).

Cancer

Sodium hypochlorite was not carcinogenic to rats or mice in chronic drinking water studies; thus, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

Sodium hypochlorite does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium hypochlorite is very toxic to aquatic organisms. The acute and subacute oral toxicity of sodium hypochlorite to birds are of low concern.

B. Aquatic Toxicity

A number of studies that have been conducted on the toxicity of sodium hypochlorite (or calcium hypochlorite) of aquatic organisms. A comprehensive summary of these studies is beyond the scope of this dossier.

In developing a water quality guideline for chlorine, ANZECC reviewed the literature on the effects of the following chemicals: chlorine gas (Cl_2) bubbled in water, sodium hypochlorite or hypochlorous acid; and ammonium sulfate or chloride and NaOCl at various combinations (molar ratios, pH values) to form monochloramine or dichloramine (ANZECC and ARMCANZ, 2000). The summary of the data measured as total residual chlorine (µg Cl/L) for freshwater fish and invertebrates is as follows:

Freshwater fish

The 24-96 hour LC_{50} values for seven species were 70- 840 µg/L. Two of the values for *O. mykiss* were 14 and 29 µg/L (Basch et al., 1971).

Freshwater crustaceans

The 24-48 LC_{50} values for three species of *cladocerans* were 12-16 µg/L. Two of the 48-hour LC_{50} values were 5 and 6 µg/L, measured under a continuous flow of test solution (Taylor, 1993).

The chronic NOEC from a 10-day *C. dubia* immobilisation study was 48 µg/L. In another chronic test, the NOEC of a 10-day *C. dubia* reproductive impairment test was 48 µg/L (Manning et al., 1996).

Freshwater Mollusc

The 24-48 hour LC_{50} values in one *Nitocris* species was 7,700 to 15,600 µg/L. The chronic 168-hour LC_{50} value for a periphyton was 32 µg/L.

Other species

The 24-48 LC_{50} values for the freshwater annelid *Aelosoma headleyi* were 1,680 to 3,200 µg/L. The 24-48 hour LC_{50} values for three species of insects were 710 to 1,350 µg/L. The 48-hour LC_{50} values for the freshwater rotifer *Philodina acuticornis* were 50 to 100 µg/L.

C. Terrestrial Toxicity

The acute oral LD_{50} value of sodium hypochlorite (12.5% solution) to bobwhite quail is >2,510 mg/kg (ECHA). [Kl. score = 2]

The 8-day oral LC_{50} value of sodium hypochlorite (12.5% solution) to bobwhite quail and mallard duck is >5,620 ppm (ECHA). [Kl. score = 2]

D. Calculation of PNEC

PNEC water

The ANZECC water quality guideline (ANZECC and ARMCANZ, 2000) used acute and chronic laboratory toxicity data for the derivation of a trigger value for chlorine. The guideline for freshwater is: “A freshwater moderate trigger value of 3 µg Cl/L measured as total residual chlorine was derived using the statistical distribution method with 95% protection. This figure was obtained from the application of the default ACR of 10 instead of the empirical ACR of 2.7 from the geometric mean of 8 figures. The smaller ACR would have resulted in a value not protective of some species under continuous exposure to chlorine for at least 48 hours”.

PNEC sediment

No experimental toxicity data on sediment organisms are available. K_{ow} and K_{oc} parameters do not readily apply to inorganics, such as sodium hypochlorite. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sed}$. Based on its properties, no adsorption of sodium

hypochlorite to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

PNEC soil

No experimental toxicity data on soil organisms are available. The environmental distribution of sodium hypochlorite is dominated by its water solubility. Sorption of sodium hypochlorite should probably be regarded as a reversible situation, *i.e.*, the substance is not tightly nor permanently bound. K_{oc} and K_{ow} parameters do not readily apply to inorganics, such as sodium hypochlorite. Thus, the equilibrium partitioning methods cannot be used to calculate the $PNEC_{soil}$. Based on its properties, sodium hypochlorite is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sodium hypochlorite is an inorganic salt that dissociates completely in water to sodium (Na^+) and hypochlorite (ClO^-) ions. Biodegradation is not applicable to these inorganic ions; For the purposes of this PBT assessment, the persistent criteria are not considered applicable to this inorganic salt.

As an inorganic salt, neither sodium hypochlorite nor its dissociated ions are expected to accumulate. Thus, sodium hypochlorite does not meet the criteria for bioaccumulation.

The lowest NOEC from chronic aquatic toxicity studies is <0.1 mg/L in invertebrates. Thus, sodium hypochlorite meets the criteria for toxicity.

The overall conclusion is that sodium hypochlorite is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, sodium hypochlorite does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for sodium hypochlorite.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Sodium Hypochlorite	7681-52-9	Not a PBT	No	No	NA	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ACR	Acute to chronic ratio
AICS	Australian Inventory of Chemical Substances
ANZECC	Australian and New Zealand Environment and Conservation Council
ARMCANZ	Agriculture and Resource Management Council of Australia and New Zealand
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EU	European Union
g	gram
IUPAC	International Union of Pure and Applied Chemistry
KI	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
LD	lethal dose
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mL	millilitre
mPa.s	millipascal second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration

ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TRC	total residual chlorine
UV	ultraviolet
µg/L	micrograms per litre

Qualitative and Quantitative Tier 3 Assessment

Tributyl Tetradecyl Phosphonium Chloride

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

Tributyl tetradecyl phosphonium chloride (TTPC) is a component in hydraulic fracturing fluid systems used in stimulation activities. Hydraulic fracturing fluid systems comprise water and chemical additives (including a proppant) blended at the surface of the well lease and injected down the cased well to improve formation permeability, enhancing the gas flow towards the well. The chemical additives are also used to assist well completion by preparing the well or maintain the gas flow to the well (i.e., prevent the swelling of clays within the target hydrocarbon formation).

The purpose and maximum quantity for this chemical in the fluid system is summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Hydraulic Fracturing Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
Tributyl tetradecyl phosphonium chloride (TTPC)	81741-28-8	biocide	0.00276%

[1] Volume Percent in Treatment (%)
CAS No = Chemical Abstracts Service Number

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 1**. TTPC is not a carcinogen, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
Tributyl tetradecyl phosphonium chloride (81741-28-8)	90-day rat drinking water	Clinical signs; decreased body weight; decreased food, water consumption	8.66	1,000	0.009	0.03

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicity reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effect concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
Tributyl tetradecyl phosphonium chloride (81741-28-8)	Acute algae	0.019	1,000	1.9×10^{-5}

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
Tributyl tetradecyl phosphonium chloride (81741-28-8)	[a]	-	-	13

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
Tributyl tetradecyl phosphonium chloride (81741-28-8)	[a]	-	-	11.5

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

TTPC is a non-oxidising biocide. Information on TTPC in this dossier has been obtained from BWA™ Water Additives, a producer of TTPC. BWA™ Water Additives produces a 5% or 50% aqueous solution of TTPC, which is sold under the product names Bellacide® 355 and Bellacide® 350, respectively. TTPC is classified as a phosphonium cationic surfactant. The molecular structure of TTPC is presented in **Figure 1**.

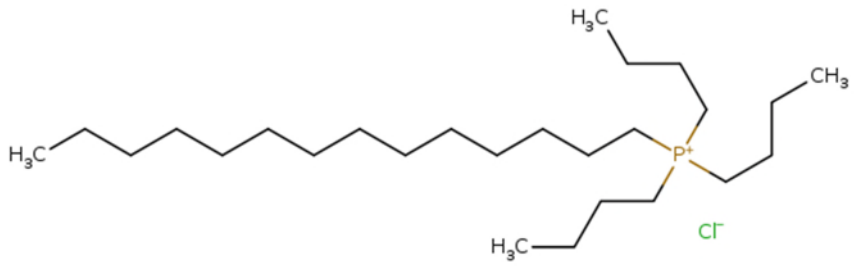

Figure 1 Molecular Structure of TTPC[2]

TTPC is stable over a wide pH range and is not susceptible to photodegradation. TTPC is biodegradable, but not readily biodegradable. It will strongly adsorb to soil and sediment. TTPC is not expected to bioaccumulate.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for TTPC is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that TTPC is not a PBT substance.

Human Health Hazards

TTPC exhibits moderate acute toxicity by the oral route, but is highly toxic by the inhalation route. It is corrosive to the skin and eyes, but it is not a skin sensitiser.

No systemic toxic effects were noted in a 90-day rat drinking water study. In rats, developmental toxicity was shown to occur at oral dose levels that were not maternally toxic; whereas, in rabbits, developmental toxicity occurred only at maternally toxic doses. TTPC was not mutagenic in a bacterial reverse mutation (Ames) test. There are no carcinogenicity studies on TTPC.

A 90-day rat drinking water study has been conducted on a product containing TTPC. Based on a review of this study, toxicological reference values were derived for TTPC. The drinking water guideline value derived for TTPC using the non-carcinogenic oral RfD is 0.03 mg/L.

TTPC may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

[2] Source https://chem.nlm.nih.gov/chemidview/image/81741-28-8?size=3

There is low potential for human receptors to be exposed to TTPC in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of stimulation fluid chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

TTPC has a very high acute toxicity concern to aquatic organisms, namely fish, invertebrates and algae. To birds, TTPC is highly toxic on an acute basis and slightly toxic on a subacute dietary basis. Under typical environmental conditions, the chemical is not readily biodegradable. However, it has a low potential for bioaccumulation.

Experimental toxicity data on water organisms was available for three trophic levels to calculate a PNEC for water. However, there are no toxicity data for soil or sediment-dwelling organisms. Therefore, PNECS for soil and sediment were calculated using the equilibrium partitioning method.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

1. Aquatic ecological receptors within Dawson River downstream of the release point
2. Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream

agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released produced water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to TTPC that may occur during hydraulic fracturing and work over activities. The risk characterisation evaluates the toxicity of this chemical and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Exposure Point Concentration Calculations

A quantitative mass balance calculation was undertaken to estimate the potential concentrations of stimulation chemicals containing TTPC within diluted produced water. For the mass balance calculation, vendor disclosure forms were used to determine the percentage of TTPC in the pre-injection fluid. **Table 6** presents the estimated pre-injection fluid concentration.

Table 6 Mass Balance Estimates for TTPC

Chemical Name	CAS No.	Estimated Pre-injection fluid concentration (mg/L)
Tributyl tetradecyl phosphonium chloride (TTPC)	81741-28-8	0.28

CAS No = Chemical Abstracts Service Number
mg/L = milligram per litre

The mass balance of TTPC was then used to estimate potential EPCs for the evaluation of releases of treated water to the Dawson River. The potential EPCs have been conservatively estimated.

First, an estimated chemical concentration in the produced water from a recently hydraulically fractured well was calculated assuming 20% of the mass returned in the flowback water to the surface at a point in time and was conservatively diluted with 150% of the injected volume of return water. The water from recently hydraulic fractured wells (10% of volume) was diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of these constituents. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. The biodegradation information was obtained from the OECD ready tests (OECD, 1992) that were developed as a first-tier testing scheme to provide preliminary screening of organic chemicals. The ready tests are stringent screening tests that are conducted under aerobic conditions in which a high concentration of the test substance is used, and biodegradation is measured by non-specific parameters including dissolved organic carbon, biochemical oxygen demand and carbon dioxide production. **Attachment 2, Table 1** includes the environmental fate information that was used to assess biodegradation of the chemical.

The concentrations in the water feed pond were then further reduced by a factor of 99% to account for efficiencies in the WMF system.

Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*. This dilution factor is far less than the dilution that would occur (>1,500 fold) based on a maximum release rate of 18 ML/day and a Dawson River average low flow of 28,000 ML/day.

These estimated surface water EPCs were used to derive EPCs for sediment using the equilibrium partitioning method. **Attachment 2, Table 1** includes the equation and environmental fate information used to derive the sediment EPC.

Release Scenario Assessment

There is no potentially complete exposure pathway to sources of drinking water; however, as a conservative measure, the theoretical concentrations for the release scenarios were compared to human health toxicity-based screening levels to screen for potential effects as a result of a release to surface water used as a drinking water source. The results of this comparison, including the ratio of exceedance of screening levels, is presented in **Attachment 2, Table 2**. As detailed in the table, the risk ratio did not exceed the target level of 1 for any of the scenarios.

Theoretical concentrations were also compared to the PNEC for aquatic receptors. **Attachment 2, Table 3** presents the results of this comparison, including the ratio of exceedance of screening levels. As detailed in the table, the risk ratio did not exceed the target level of 1 for any of the scenarios.

The primary land use within the development area is agricultural (grazing on improved or unimproved pastures), and it is sparsely populated. To further evaluate potential risks to non-MNES receptors (mammals and avian), additional quantitative analysis of the managed releases to Dawson River was conducted.

Terrestrial receptors evaluated for exposure to Dawson River discharge include domesticated livestock, large mammalian wildlife and small mammalian wildlife. Beef cattle were used to evaluate domesticated livestock, kangaroos were evaluated for large mammalian wildlife, and dingos were evaluated for small mammalian wildlife. The cattle egret was selected to evaluate avian exposures. Exposure assumptions, TRVs and total intake calculations are detailed in **Attachment 2, Tables 4, 5, 6 and 7**. **Attachment 2, Table 4** presents the calculated risk estimates for the kangaroo. **Attachment 2, Table 5** presents the calculated risk estimates for the dingo. **Attachment 2, Table 6** presents the calculated risk estimates for the cattle. **Attachment 2, Table 7** presents the calculated risk estimates for the cattle egret. As indicated in the tables, the calculated HQ for TTPC did not exceed the risk threshold level of 1 for any of the scenarios evaluated.

Cumulative Impacts

The potential for cumulative impacts associated with chemicals used during stimulation activities is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), TTPC does meet the criteria for persistence but does not meet the criteria for bioaccumulation. Further, estimated concentrations in surface water and sediment were less than PNECs. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 7** below provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 7 Evaluation of Uncertainty – TTPC

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentrations of COPCs in residual stimulation fluids were estimated based on previous operations and may not accurately estimate the concentrations of COPCs in the future. Detailed discussions with Santos occurred to identify a conservative estimate of the COPC; however, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may overestimate or underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Exposure Assessment	The use of the food consumption relationship with body weight for mammalian and avian receptors.	Low to Medium	Low to medium potential to underestimate or overestimate risk
Toxicity Assessment	The use of acute toxicity data (rather than chronic toxicity data) to calculate PNECs for water and no data to calculate PNECs for soil and sediment.	Medium	Medium to high potential to overestimate risks.
Toxicity Assessment	The use of toxicity values in a risk assessment is based on extrapolations from animal data, adjust factors for inherent uncertainty in the toxicological estimate and use of surrogate toxicity criteria	Low	Low potential to underestimate risk
Toxicity Assessment	The use of LOAEL/NOAEL for calculation of the TRVs	Low to Medium	Low to medium potential to underestimate or overestimate risk
Toxicity Assessment	The use of the allometric scaling method to estimate the population-level effects on wildlife based on individual level of exposures.	Low to Medium	Low to medium potential to underestimate or overestimate risk

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Attachment 1 Risk Assessment Dossier

TRIBUTYL TETRADECYL PHOSPHONIUM CHLORIDE

This dossier on tributyl tetradecyl phosphonium chloride (TTPC) presents the most critical studies pertinent to the risk assessment of TTPC in its use in hydraulic fracturing fluids. This dossier does not represent an exhaustive or critical review of all available data. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – TTPC was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. However, TTPC was assessed as a tier 3 chemical for acute toxicity and as a tier 3 chemical for chronic toxicity. Therefore, TTPC is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

TTPC is a non-oxidising biocide. TTPC is stable over a wide pH range and is not susceptible to photodegradation. TTPC is biodegradable, but not readily biodegradable. It will strongly adsorb to soil and sediment. TTPC is not expected to bioaccumulate. TTPC has a very high acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Tributyl(tetradecyl)phosphonium chloride

CAS RN: 81741-28-8

Molecular formula: $C_{26}H_{56}PCl$

Molecular weight: 435.15 g/mol

Synonyms: Tributyl tetradecyl phosphonium chloride; TTPC; tri-n-butyltetradecylphosphonium chloride; Bellacide 350; Bellacide 355

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of TTPC

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Clear, colourless liquid	4	BWA Water Additives (2016)
Boiling Point	100°C*	4	BWA Water Additives (2016)
Specific Gravity	0.98 – 1.00 @ 20°C	4	BWA Water Additives (2016)
Partition Coefficient (log K_{ow})	2.45	4	BuruEnergy
Viscosity	55-65 mm^2/s @ 25°C	4	BWA Water Additives (2016)

*5% aqueous solution of TTPC

TTPC is a non-oxidising biocide. Information on TTPC in this dossier has been obtained from BWA™ Water Additives, a producer of TTPC. BWA™ Water Additives produces a 5% or 50% aqueous solution of TTPC, which is sold under the product names Bellacide® 355 and Bellacide® 350, respectively.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for TTPC.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	.No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

TTPC is stable over a wide pH range and is not susceptible to photodegradation. TTPC is biodegradable, but not readily biodegradable. It will strongly adsorb to soil and sediment. TTPC is not expected to bioaccumulate.

B. Abiotic Degradation

Hydrolysis

TTPC is stable over a wide pH range (BuruEnergy). [Kl. score = 4]

Photolysis

TTPC is not susceptible to photodegradation. (BuruEnergy). [Kl. score = 4]

C. Biodegradation

TTPC was not readily biodegradable in an OECD 301 test (BuruEnergy). [Kl. score = 4]

A die-away [simulation] test was conducted with radiolabelled TTPC for 168 hours at concentration of 0.31 mg/L. The first-order rate constant was 0.69/hour and the half-life was 6.6 hours. After 24 and 168 hours, degradation was >81% and >98%, respectively (BuruEnergy). [Kl. score = 4]

TTPC was evaluated in a simulation test over a 40-day period using double ^{14}C labelled TTPC. In activated sludge, there was >40% degradation after 30 days with 50 ppb TTPC and >30% degradation after 7 days with 5 ppb TTPC. In river water, there was >20% after 35 days with 5 ppb TTPC. In sea water, there was >30% degradation after 35 days with 5 ppb TTPC (BuruEnergy). [Kl. score = 4]

D. Environmental Distribution

Adsorption/desorption

TTPC strongly adsorbs to soil. In a study involving three different soil types (sand, silt and clay), 93 to 96% of TTPC adsorbed to soil (BuruEnergy). [Kl. score = 4]

No experimental studies are available for determining the K_{oc} of TTPC. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value for TTPC using the MCI method is 4.555×10^7 L/kg.

E. Bioaccumulation

No bioaccumulation studies are available on TTPC. TTPC is not expected to bioaccumulate based on the experimental log K_{ow} of 2.45 (Buruenergy). [Kl. Score = 4]

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

TTPC exhibits moderate acute toxicity by the oral route, but is highly toxic by the inhalation route. It is corrosive to the skin and eyes, but it is not a skin sensitiser. No target organ effects were noted in a 90-day rat drinking water study. TTPC was not mutagenic in a bacterial reverse mutation (Ames) test. There are no carcinogenicity studies on TTPC. In rats, developmental toxicity was shown to occur at oral dose levels that were not maternally toxic; whereas, in rabbits, developmental toxicity occurred only at maternally toxic doses.

B. Acute Toxicity

An oral LD_{50} in rats for Bellacide 350 (50% aq. solution of TTPC) was reported to be >1,002 mg/kg (BWA Water Additives, 2011) [Kl. score = 4]. An oral LD_{50} in rats for Bellacide 355 (5% aqueous solution of TTPC) was reported to be >4,000 mg/kg (BWA Water Additives, 2016). [Kl. score = 4]

The 4-hour inhalation LC_{50} in male and female rats for a 50% aq. solution of TTPC was <0.05 mg/L (aerosol). The mass median aerodynamic diameter for the aerosol was 1.93 µm (Cytec, 2012) [Kl. score = 1]. The 1-hour inhalation LC_{50} in male and female rats for a 50% aq. solution of TTPC is 0.227 mg/L (aerosol). The mass median aerodynamic diameter for the aerosol was 1.92 µm (Cytec, 2013) [Kl. score = 1].

C. Irritation

Both Bellacide 350 (50% aq. solution TTPC) and Bellacide 355 (5% aq. solution TTPC) are considered to be corrosive to the skin and eyes (BWA Water Additives, 2011 and 2015). [Kl. score = 4]

D. Sensitisation

TTPC is not considered to be a skin sensitiser (BWA Water Additives, 2011 and 2015). [Kl. score = 4]

E. Repeated Dose Toxicity

Oral

A 90-day rat drinking water study has been conducted on a product containing TTPC. The LOAEL for the active ingredient (TTPC) is 27.2 and 32.3 mg/kg-day in males and females, respectively, based on various clinical signs and significantly reduced body weights, feed and water consumption. The NOAEL for this study is 8.66 mg/kg-day (USEPA, 2006). [Kl. score = 2]

Inhalation

No data are available.

Dermal

No data are available.

F. Genotoxicity

In vitro Studies

TTPC was not mutagenic in a reverse mutation bacterial (Ames) test (BWA Water Additives, 2015). [Kl. score = 4]

In vivo Studies

No studies are available.

G. Carcinogenicity

No studies are available.

H. Reproductive Toxicity

No studies are available.

I. Developmental Toxicity

Female Tif:RAIf(SPF) rats were dosed by oral gavage with 0, 20, 60 or 120 mg/kg Belclene® [50% active ingredient: TTPC] during gestational days (GD) 6-15. In the high-dose group, there were two possible treatment-related spontaneous deaths (GD 9 and 14) and another death on GD 15 due to an intubation error. Clinical signs included dyspnea in one mid-dose and four high-dose animals, and vaginal bleeding in one mid-dose female on GD 15. In the high-dose group, maternal body weight gain was significantly lower during the treatment period (GD 6-15) and throughout the gestational period (GD 0-20). Mean food consumption was significantly reduced during GD 6-11 for both the mid- and high-dose animals. The number of females with implantations and the number of implantations/females were similar across all groups. Embryonic and fetal deaths were similar between treated and control groups. There were no soft tissue changes. There was an increased incidence of incomplete ossification of the 5th sternebra in the mid- and high-dose groups. The NOAELs for maternal and developmental toxicity for the active ingredient TTPC in this study is 30 and 10 mg/kg-day, respectively (USEPA, 2006). [Kl. score = 2]

Female chinchilla rabbits were dosed by oral gavage with 0, 7.5, 22.5 or 45 mg/kg Belclene® [50% active ingredient: TTPC] during GD 6-18. In the mid- and high-dose groups, body weight gain was significantly reduced during GD 6-18 and feed consumption was reduced during GD 6-11. Fetal body weights were significantly reduced in the mid-(males only) and high-dose groups. There was also an increased incidence of delayed ossification of the hindlimb phalangeal nuclei in the mid- and high-dose groups. The NOAEL for maternal and developmental toxicity for the active ingredient TTPC in this study is 3.75 mg/kg-day (USEPA, 2006). [Kl. score = 2]

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for TTPC follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

<u>Oral</u>

The NOAEL from a rat 90-day drinking water study based on various clinical signs and significantly reduced body weight and reduced feed and water consumption is 8.66 mg a.i./kg-day (USEPA, 2006). This NOAEL will be used to derive the oral reference dose.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 8.66/(10 x 10 x 1 x 10 x 1) = 8.66/1000 = 0.009 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.009 x 70 x 0.1)/2 = 0.03 mg/L

Cancer

No carcinogenicity studies are available on TTPC. Thus, a cancer reference dose was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

TTPC does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

TTPC has a very high acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on TTPC.

Table 3 Acute Aquatic Toxicity Studies on TTPC

Test Species	Endpoint	Results (µg/L)	Klimisch score	Reference
Bluegill sunfish	96-hour LC_{50}	58.6	2	ECOTOX
Common Carp	96-hour LC_{50}	87	2	ECOTOX
Rainbow trout	96-hour LC_{50}	490	2	ECOTOX
Rainbow trout	96-hour LC_{50}	200	2	ECOTOX
Daphnia magna	48-hour EC_{50}	25.2	2	ECOTOX
Selenastrum capricornutum	72-hour EC_{50}	19	4	BuruEnergy

Chronic Studies

No studies are available.

C. Terrestrial Toxicity

Table 4 lists the avian toxicity studies conducted on TTPC.

Table 4 Avian Toxicity Studies on TTPC

Test Species	Endpoint	Results	Kl. score	Reference
Bobwhite Quail	8-day dietary	LC_{50}: 4,215 ppm NOEL: 1,980 ppm	2	ECOTOX
Mallard Duck	8-day dietary	LC_{50}: 3,663 ppm NOEL: 1,780 ppm	2	ECOTOX
Mallard Duck	14-day oral gavage	LD_{50}: 232 mg/kg NOEL: <178 mg/kg	2	ECOTOX

D. Calculation of PNEC

The PNEC calculations for TTPC follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute EC_{50} values are available for fish (58.6 µg/L), *Daphnia* (25 µg/L) and algae (19 µg/L). No chronic toxicity studies are available on TTPC. On the basis that the data consists of short-term results from three trophic levels, an assessment factor of 1,000 has been applied to the effect concentration of 19 µg/L for algae. The $PNEC_{water.}$ is calculated to be 0.019 µg/L (1.9×10^{-5} mg/L).

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 12,982 µg/kg (13.0 mg/kg) sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (874{,}561/1280) \times 1000 \times 0.019$
$= 12{,}982$

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 1{,}822{,}000/1000 \times 2400]$
$= 874{,}561$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 45{,}550{,}000 \times 0.04$
$= 1{,}822{,}000$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for TTPC calculated from EPISuite™ using the MCI method is 4.555×10^7 L/kg.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 11,539 µg/kg (11.5 mg/kg) soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (911{,}000/1500) \times 1000 \times 0.019$
$= 11{,}539$

Where:
Kp_{soil} = soil-water partition coefficient (m3/m3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 45{,}550{,}000 \times 0.02$
$= 911{,}000$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for TTPC calculated from EPISuite™ using the MCI method is 4.555×10^7 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

In a simulation test using river water, there was >20% after 35 days; however, no information is available on longer time points. TTPC is not readily biodegradable; thus it meets the screening criteria for persistence.

The log K_{ow} for TTPC is 2.45. Thus, TTPC does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies available on TTPC. The lowest acute EC_{50} value for TTPC is <1 mg/L in algae. Thus TTPC meet the criteria for toxicity.

Therefore, TTPC is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, TTPC does meet

the criteria for persistence but does not meet the criteria for bioaccumulation. Further evaluation of cumulative impacts is provided in the quantitative risk assessment.

No other characteristics of concern were identified for TTPC.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Tributyl tetradecyl phosphonium chloride	81741-28-8	Not a PBT	No	No	Yes	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 3 – Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRYNOYMS

A. References

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B. Abbreviations and Acronyms

^{o}C	degrees Celsius
a.i./kg-day	active ingredient per kilogram per day
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
GD	gestational day
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration

LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/kg-day	milligrams per kilogram per day
mg/L	milligrams per litre
mm^2/s	square millimetres per second
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEL	no observed effect level
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppb	parts per billion
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	reference dose
SGG	Synthetic Greenhouse Gases
TTPC	tributyl tetradecyl phosphonium chloride
USEPA	United States Environmental Protection Agency
µg/kg	micrograms per kilogram
µg/L	micrograms per litre
µm	micrometre

Attachment 2 Risk Characterisation Tables

Attachment 2, Table 1
Summary of Exposure Point Concentrations

Chemical	CAS No.	Estimated concentration in pre-injection fluid systems (mg/L)	Half-Life (days)	Estimated Flowback Concentration (mg/L)[1]	Estimated Concentration in Combined Balance Water Feed Pond to WMF (mg/L)[2]		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[3]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[4]		Estimated Concentration in Dawson River Sediment (mg/kg)[5]	
					Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)	
					0	30	0	30	0	30	0	30
Tributyl tetradecyl phosphonium chloride	81741-28-8	2.82E-01	1.50E+02	3.76E-02	3.76E-03	3.27E-03	3.76E-05	3.27E-05	7.52E-07	6.55E-07	5.14E-01	4.48E-01

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated flowback concentration in pond influent (150% of injected fluid volume) per coal seam per 20% of mass returned calculated using equation: Pond Influent = FBconcentration (mg/L)/ FB dilution 150% x percent mass returned (mg/L)
2) Estimated flowback concentration was multiplied by a factor of 10% to account for dilution in the water feed pond (90:1) due to the aggregation of produced water from other wells which were not recently hydraulically fractured into the same pond.
3) Concentrations in the water feed pond were further reduced by a factor of 99% to account for efficiencies in the WMF system.
4) A dilution factor of 50 was assumed within the approved mixing zone.
5) $EPC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times EPC_{water}$
Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = treated water EPC
$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]
$Kp_{sed} = K_{oc} \times f_{oc}$
Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg), chemical-specific value found in dossier provided in Attachment 1.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

Attachment 2, Table 2
Comparison of Theoretical Concentrations of COPCs to Drinking Water Guidelines

Permeate Pond								
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[1]		Drinking Water Screening Level (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30
Tributyl tetradecyl phosphonium chloride	81741-28-8	3.76E-05	3.27E-05	7.52E-07	6.55E-07	3.00E-02	2.5E-05	2.2E-05

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 2, Table 3
Comparison of Theoretical Concentrations of COPCs to PNECs (Water and Sediment)

Permeate Pond														
Chemical	CAS No.	Estimated Concentration in Permeate after 99% treatment efficiency by RO plant (mg/L)[1]		Estimated Concentration in Dawson River (Treated Water Release) (mg/L)[1]		PNEC aquatic (mg/L)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)		Estimated Concentration in Dawson River Sediment (mg/kg)[1]		PNEC sediment (mg/kg)	Ratio of COPC Concentrations and Screening Criteria (Ratio greater than one = unacceptable potential risk)	
		Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)		Temporal Scenario (days)			Temporal Scenario (days)	
		0	30	0	30		0	30	0	30		0	30
Tributyl tetradecyl phosphonium chloride	81741-28-8	3.76E-05	3.27E-05	7.52E-07	6.55E-07	1.90E-05	3.96E-02	3.4E-02	5.14E-01	4.48E-01	1.30E+01	4.0E-02	3.4E-02

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility

1) Estimated concentrations derived in Table 1.

Attachment 2, Table 4
Risk Estimates for Cattle Egret - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Avian NOAELt [1]	Avian NOAEL Test Animal		Avian Receptor Cattle Egret	
			Animal	Body Weight (kg)		Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Tributyl tetradecyl phosphonium chloride	81741-28-8	8.66E+00	Rat	3.50E-01	1980.0	Bobwhite Quail	0.178	3.90E-01	1.6E+03

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.03	(c)
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	0.39	Siegfried, 1969
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
W.R. Siegfried (1969) Energy Metabolism of the Cattle Egret, ZoologicaAfricana, 4:2, 265-273, DOI: 10.1080/00445096.1969.11447375
c/ Drinking water ingestion rate (WIR) based on the allometric relationship developed by Calder and Braun (1983), where WIR (L/day) = 0.059 x BW (Kg)$^{0.67}$

Constituent Name	CAS No.	EPC [1] Day 0	EPC [1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Tributyl tetradecyl phosphonium chloride	81741-28-8	7.5E-07	6.5E-07	1.6E+03	1.1E-09	6.8E-13	9.7E-10	5.9E-13

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365^{\ days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 2, Table 5
Risk Estimates for Kangaroo - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL Test Animal		Mammal Kangaroo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Tributyl tetradecyl phosphonium chloride	81741-28-8	8.66E+00	Rat	3.50E-01	2.50E+01	2.98E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	3	Fleming, 2001
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	25	Fleming, 2001
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram
b/ References:
BPJ - Best Professional Judgement
Fleming, 2001
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Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Tributyl tetradecyl phosphonium chloride	81741-28-8	7.5E-07	6.5E-07	3.0E+00	1.7E-09	5.8E-10	1.5E-09	5.1E-10

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 2, Table 6
Risk Estimates for Dingo - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Dingo	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Tributyl tetradecyl phosphonium chloride	81741-28-8	8.66E+00	Rat	3.50E-01	1.30E+01	3.51E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weighttest}{Body\ Weightreceptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	0.75	Dawson, 1995
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	13	Dawson, 1995
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
Dawson, 1995
Dawson, Terence J. (1995). Kangaroos: Biology of the Largest Marsupials. Cornell University Press, Ithaca, New York. Second printing: 1998. ISBN 0-8014-8262-3.

Constituent Name	CAS No.	EPC[1] Day 0	EPC[1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Tributyl tetradecyl phosphonium chloride	81741-28-8	7.5E-07	6.5E-07	3.5E+00	8.3E-10	2.4E-10	7.2E-10	2.1E-10

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Attachment 2, Table 7
Risk Estimates for Cattle - Dawson River Release

Constituent Name	CAS No.	Mammal NOAELt	Mammal NOAEL		Mammal	
			Test Animal		Cattle	
			Animal	Body Weight (kg)	Body Weight (kg)	Derived TRV
Tributyl tetradecyl phosphonium chloride	81741-28-8	8.66E+00	Rat	3.50E-01	4.54E+02	1.44E+00

Notes:
NOAELt = No observed adverse effect level test animal
kg = kilogram
NA = not applicable
TRV = toxicity reference value
1/ If an avian NOAEL was not available, the mammal NOAEL was used to derive the TRV for the avian receptor.

$$Derived\ TRV = NOAEL_{test} * \left(\frac{Body\ Weight test}{Body\ Weight receptor}\right)^{(1/4)}$$

Exposure Route	Parameter Code	Parameter Definition	Units (a)	Parameter Value	Source (b)
Ingestion	IR	Ingestion rate	l/day	86	API, 2004
	EF	Exposure frequency	day/yr	7	BPJ
	ED	Exposure duration	yr	1	BPJ
	BW	Body weight	kg	454	API, 2004
	AT-NC	Averaging time - noncancer	days	365	BPJ

Notes:
a/ Units:
l/day = litres per day
day/yr = days per year
yr = year
kg = kilogram

b/ References:
BPJ - Best Professional Judgement
API, 2004
API. (2004). Risk-Based Screening Levels for the Protection of Livestock Exposed to Petroleum Hydrocarbons, Regulatory Analysis and Scientific Affairs No. 4733 July 2004.

Constituent Name	CAS No.	EPC [1] Day 0	EPC [1] Day 30	Toxicity	Total Intake (mg/kg/day)	Hazard Quotient	Total Intake (mg/kg/day)	Hazard Quotient
		CW (mg/l)	CW (mg/l)	TRVs	Day 0	Ingestion	Day 30	Ingestion
Tributyl tetradecyl phosphonium chloride	81741-28-8	7.5E-07	6.5E-07	1.4E+00	2.7E-09	1.9E-09	2.4E-09	1.6E-09

Notes:
CW = concentration in water
EPC = exposure point concentration
mg/kg/day = milligrams per kilograms per day
mg/l = milligrams per liter
NA = not available/applicable
TRV = toxicity reference value
1/ EPC is estimated concentration in Dawson River in Table 1 for Day 0 and Day 30

$$Total\ Intake = \frac{EPC\ \times IR\ \times EF\ \times ED}{BW\ \times ED\ x\ 365\ ^{days}/_{year}}$$

$$Hazard\ Quotient = \frac{Total\ Intake\ \left(\frac{mg}{kg-day}\right)}{TRV\ \left(\frac{mg}{kg-day}\right)}$$

Qualitative and Quantitative Tier 3 Assessment

2,2-Dibromo-3-Nitrilopropionamide

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), the assessment for this Tier 3 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No-Effects Concentrations (PNECs) for water and soil; and, completing a qualitative and quantitative assessment of risk. Each of these components is detailed within this attachment.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

2,2-Dibromo-3-nitrilopropionamide (DBNPA) is a component in a Water Management Facility (WMF) product used as a biocide. Process and usage information for this chemical is included in **Attachment 1** and summarised in **Table 1**.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 1 Water Management Facility Chemicals – Tier 3 Chemicals

Chemical Name	CAS No.	Use	Approximate Quantity Stored On-Site (plant available storage)
DBNPA Sodium Bromide Dibromoacetonitrile	10222-01-2 7647-15-6 3252-43-5	Biocide	2 x 1000 L (IBC)

CAS No = Chemical Abstracts Service Number
CIP = clean-in-place
IBC = intermediate bulk container
L = litre

The assessment of toxicity of this chemical was used to develop initial screening criteria for human health exposure scenarios and is presented in the risk assessment dossier provided in **Attachment 2**. DBNPA is not a carcinogen; and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
DBNPA (10222-01-2)	90-day rat oral gavage	Mortality, weight loss, dyspnea	5	1000	0.005	0.02

CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level
Refer to **Attachment 2** for information on the key studies selected for oral reference dose and drinking water level development.

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna for the chemical. The qualitative assessment focuses on the aquatic invertebrate and fish species within the surface water resources, and the soil flora and fauna associated with releases to the soil. The quantitative assessment includes evaluating the potential risks to these same aquatic and soil ecological receptors, in addition to higher trophic level organisms such as livestock and terrestrial wildlife.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment are developed to assess aquatic receptors, and PNECs for soil are developed for terrestrial receptors.

Table 3 presents the chemical, endpoint, no observed effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are

detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 2** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
DBNPA (10222-01-2)	Invertebrates	0.05	50	0.001

EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
DBNPA (10222-01-2)	[a]	-	-	0.0015

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observed effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 3 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
DBNPA (10222-01-2)	[a]	-	-	0.00077

[a]Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 2** for information on the development of PNECs listed above.

A detailed assessment of the potential risks posed by this Tier 3 chemical is provided in the following sections.

General Overview

DBNPA is an organic bromine compound and is a reaction product of bromine (CAS# 7726-95-6) and cyanoacetamide (CAS# 107-91-5). The molecular structure of DBNPA is presented in **Figure 1**.

Figure 1 Molecular Structure of DBNPA[2]

DBNPA is biodegradable at expected environmental exposure concentrations, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment. Hydrolysis of DBNPA is expected to be the dominant path of environmental degradation. The substance is also susceptible to photolysis, with half-lives ranging from 0.4 hours to 14.8 hours, depending on pH. In both anaerobic and aerobic metabolism studies, half-lives of less than 4 hours were measured for DBNPA; loss was due to both hydrolysis and biodegradation.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for DBNPA is included in the dossier provided in **Attachment 2**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that DBNPA is not a PBT substance.

Human Health Hazards

DBNPA is acutely toxic by the oral and inhalation routes, but not by the dermal route. It is corrosive to the skin and eyes. DBNPA is a skin sensitiser. Inhalation exposure of an aerosol or mist can cause respiratory irritation.

Repeated oral exposures in rats showed some evidence of kidney toxicity. There was no evidence of systemic toxicity following repeated dermal exposures. It is not genotoxic or carcinogenic. It is not expected to cause reproductive or developmental effects.

Based on a review of repeated dose and developmental toxicity studies, toxicological reference values were derived for DBNPA. The drinking water guideline value derived for DBNPA using the non-carcinogenic oral RfD is 0.02 mg/L.

Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

However, there is low potential for exposure. There are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/10222-01-2

fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), data base indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Based on the environmental fate properties described in **Attachment 2** and discussed above, DBNPA hydrolyses rapidly (half-lives 5 hours) in natural waters to many degradates which continue to degrade rapidly by aerobic and anaerobic aquatic metabolism. Based on the treatment process described in **Attachment 1**, these degradates would be removed by the reverse osmosis (RO) system, with the majority directed to brine (i.e., less than 5% to permeate) and subject to further degradation. Therefore, the biocide is not expected to be a significant risk driver. As a result, this chemical was not evaluated further in permeate or brine. Therefore, exposure pathways associated with Dawson River discharge would be incomplete.

Environmental Hazards

In standard aquatic toxicity tests, DBNPA is very toxic to aquatic organisms on both an acute and chronic basis. In the acute aquatic tests, algae were found to be the most sensitive species. Fish and invertebrates were less susceptible. However, invertebrates were the most sensitive in chronic aquatic tests. DBNPA is also moderately acutely toxic to birds. Under typical environmental conditions, the chemical is expected to degrade rapidly in soil and water and does not persist in the environment. The chemical also does not bioaccumulate.

Experimental toxicity data on water organisms was available for three trophic levels to calculate PNECs. However, there are no toxicity data for sediment-dwelling or soil organisms. Therefore, the $PNEC_{sed}$ and $PNEC_{soil}$ were calculated using the equilibrium partitioning method.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream

agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

However, as discussed earlier, exposure pathways associated with Dawson River discharge would be incomplete, including those associated with MNES receptors.

Risk Characterisation

The purpose of the risk characterisation portion of the assessment is to provide a conservative estimate of the potential risk resulting from exposure to DBNPA that may occur during water treatment activities. The risk characterisation evaluates the toxicity of DBNPA and characterises the risk of the chemical assessed for specific exposure pathways identified in the previous sections.

A two-stage process is employed during risk characterization. First, risk ratios are developed for the chemical for potentially complete exposure pathways associated with applicable release scenarios. The risk ratio is calculated by dividing the exposure point concentration (EPC) by the applicable risk-based screening level (drinking water level or PNECs for aquatic and terrestrial receptors). If the ratio of exceedance of screening levels is less than 1.0, then there are no anticipated adverse effects associated with the exposure scenario evaluated. No risk / hazard reduction measures are required. There should be no need for further management controls on the chemical additional to those already in place (DoEE, 2017).

If the ratio is greater than 1.0, then further quantitative analysis is conducted. Consistent with the assessment framework, quantitative assessment of risk will consider only Tier 3 chemicals in end use determination.

Release Scenario Assessment

As previously noted, DBNPA would not be present in permeate, brine or treated water. Therefore, EPCs were not developed for releases to the Dawson River; and likewise, further quantitative analysis (i.e., calculation of hazards) for Dawson River discharge was not conducted.

Cumulative Impacts

The potential for cumulative impacts associated with water treatment chemicals is limited. Residual chemicals may be entrained within produced water and subsequently transported for water treatment at a WMF. However, these chemicals are removed by the treatment systems; and, therefore, no additional risk is provided during managed releases to Dawson River. Likewise, the presence of water treatment chemicals at the point of produced water storage or during managed releases to the Dawson River also poses no significant increase in risk.

Tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted earlier and discussed in detail in the dossier (**Attachment 2**), DBNPA does not meet the criteria for persistence or bioaccumulation.

Further, DBNPA would not be present in permeate, brine or treated water. Thus, there is negligible incremental risk posed by the use of this Tier 3 chemical and the existing management and monitoring controls are appropriate to ensure that the risk to MNES (and non MNES) receptors remains low.

Uncertainty Analysis

The procedures and assumptions used to assess potential human health risks in this Tier 3 assessment are subject to a wide variety of uncertainties. However, the presence of uncertainty is inherent in the risk assessment process, from the sampling and analysis of the chemical in environmental media to the assessment of exposure and toxicity, and risk characterisation. Accordingly, it is important to note that the risks presented within this Tier 3 assessment are based on numerous conservative assumptions in order to be protective of human health and the environment, and to ensure that the risks presented herein are more likely to be overestimated rather than underestimated.

The discussion detailed in **Table 6** provides an evaluation of uncertainty for this Tier 3 assessment, including elements previously discussed within this assessment.

Table 6 Evaluation of Uncertainty – DBNPA

Risk Characterisation Component	Description of Uncertainty	Magnitude of Uncertainty	Effect on Risk Assessment
Hazard Assessment –COPC concentrations	The concentration of DBNPA in permeate, brine or treated water was not estimated. The substance hydrolyses and rapidly biodegrades. However, there is the potential that the empirical concentrations would differ than those presented in the risk assessment.	Low	This assumption may underestimate the calculated risks to receptors, dependent on-site-specific conditions.
Toxicity Assessment	The absence of toxicity data for sediment-dwelling or soil organisms to calculate a PNEC in sediment or soil. The PNEC was calculated using the equilibrium partitioning method.	Medium	This assumption may overestimate risk.

References

AECOM. 2019. Revised Boron Site-Specific Water Quality Criterion – Dawson River Release Scheme. Letter from B. Goldsworthy and N. Lee to A. Lavery. 12 July 2019.

Australian Environmental Agency (AEA). (2009). Environmental Risk Assessment Guidance Manual for Industrial Chemicals, Commonwealth of Australia. Available: http://www.nepc.gov.au/resource/chemical-risk-assessment-guidance-manuals

Department of the Environment and Energy (DoEE). (2017). Exposure draft: Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction. Commonwealth of Australia, available at http://www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual

frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.

Attachment 1 Vendor WMF Chemicals and Exposure Point Concentration

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	%	Proper Shipping Name	Supplier	Area	Transport		Onsite Storage		Operation		Annual Usage (ROP volumes based on peak rate of 10ML/d)	Purpose / Function
							mass/volume	concentration	mass/volume	concentration	mass/volume	concentration		
Biomate MBC2881	DBNPA (2,2-Dibromo-3-Nitrilopropionamide) Sodium Bromide Dibromoacetonitrile Non-hazardous ingredients	10222-01-2 7647-15-6 3252-43-5 N/A	20-40% 2.5-10% 0.1-1% remainder	Biomate MBC2881	Suez Water Technologies and Solutions Pty Ltd	Reverse Osmosis Plant	1000L IBC		2 x 1000L (IBC)		20 mg/L	20%		biocide

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 1
Summary of Exposure Point Concentration Development
(Water Treatment Chemicals)

Product Name	Chemical Name	CAS Number	Fate	Permeate Concentration		COPC concentration in soil from release of permeate	COPC concentration in soil from 20 years of irrigation	Brine Concentration	
				(mg/L)	Permeate notes	(mg/kg)	mg/kg	(mg/L)	Brine Notes
Biomate MBC2881	DBNPA (2,2-Dibromo-3-Nitrilopropionamide)	10222-01-2	No residual	NA	Completely breaks down to carbon dioxide, ammonia and bromide ions. These degradates are removed by the RO system (95%) goes to brine, 5% stays within permeate. Residual concentrations are de minimis and full degrade in the pond.	NA	NA	NA	Completely breaks down to carbon dioxide, ammonia and bromide ions. These degradates are removed by the RO system (95%) goes to brine, 5% stays within permeate. Residual concentrations are de minimis and fully degrade in the pond.
	Sodium Bromide	7647-15-6		NA		NA	NA	NA	
	Dibromoacetonitrile	3252-43-5		NA		NA	NA	NA	
	Non-hazardous ingredients	N/A		NA		NA	NA	NA	

AVG = average
CAS = Chemical Abstracts Service
COPC = constituent of potential concern
IBC = intermediate bulk container
L = litres
mg/kg = milligrams per kilogram
mg/L = milligrams per litre
ML/d = millilitre per day
NA = not applicable
ROP = reverse osmosis process

Attachment 2 Risk Assessment Dossier

2,2-DIBROMO-3-NITRILOPROPIONAMIDE

This dossier on 2,2-dibromo-3-nitrilopropionamide (DBNPA) presents the most critical studies pertinent to the risk assessment of DBNPA in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the U.S. EPA Reregistration Eligibility Decision (RED) document on DBNPA (EPA, 1994), U.S. EPA Draft Risk Assessment for DBNPA (EPA, 2019) and the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) assessment on DBNPA (NICAS, 2016). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – DBNPA was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. However, DBNPA was assessed as a tier 3 chemical for acute toxicity and as a tier 3 chemical for chronic toxicity. Therefore, DBNPA is classified overall as a **tier 3** chemical and requires a quantitative risk assessment for end uses.

1 BACKGROUND

During water treatment, DBNPA is used as a biocide. It controls bacteria, fungi, and algae in reverse osmosis systems.

DBNPA hydrolyses under both acid and alkaline conditions and then quickly degrades to various degradates. It is biodegradable at expected environmental exposure concentrations, has a low potential for bioaccumulation, and is not expected to adsorb to soils or sediment based on the low measured K_{ow}.

DBNPA is acutely toxic by the oral and inhalation routes, but not by the dermal route. It is corrosive to the skin and eyes. DBNPA is a skin sensitiser. Inhalation exposure of an aerosol or mist can cause respiratory irritation. Repeated oral exposures in rats showed some evidence of kidney toxicity. There was no evidence of systemic toxicity following repeated dermal exposures. It is not genotoxic or carcinogenic. It is not expected to cause reproductive or developmental effects.

DBNPA is very toxic to aquatic organisms. DBNPA is also moderately acutely toxic to birds.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): 2,2-Dibromo-2-cyanoacetamide

CAS RN: 10222-01-2

Molecular formula: $C_3H_2Br_2N_2O$

Molecular weight: 241.87 g/mol

Synonyms: 2,2-Dibromo-2-cyanoacetamide; DBNPA; 2,2-dibromo-3-nitrilopropionamide

3 PHYSICO-CHEMICAL PROPERTIES

DBNPA is an organic bromine compound and is a reaction product of bromine (CAS# 7726-95-6) and cyanoacetamide (CAS# 107-91-5). Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of DBNPA

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White to "off white" colour crystalline solid	1	EPA, 2019
Melting Point	123 – 125°C @ 101.3 kPa	1	EPA, 2019
Boiling Point	Decomposes at 190°C @ 101.3 kPa	1	EPA, 2019
Density	934 -1,370 kg/m^3 (temperature not provided)	1	EPA, 2019
Vapour Pressure	0.120 Pa @ 25°C	1	EPA, 2019
Partition Coefficient (log K_{ow})	0.80-0.88 L/kg (pH not provided)	1	EPA, 2019
Water Solubility	15 g/L @ 25°C	1	EPA, 2019
Dissociation Constant (pKa)	8.24	2	EPA, 2019

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No other specific environmental regulatory controls or concerns were identified within Australia and internationally for DBNPA.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

DBNPA is biodegradable at expected environmental exposure concentrations, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment.

B. Partitioning

DBNPA is highly soluble in water. Volatilisation from water surfaces or moist soil surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant (1.9×10^{-3} Pa m^3/mol). It is also not expected to volatilise from dry soil surfaces based upon its vapor pressure (Pub Chem).

Degradation of DBNPA is extremely pH dependent with increased degradation rates observed at higher pH's. DBNPA is hydrolytically stable at pH 5 with a half-life of 67 days, and hydrolytically unstable at pH 7 and 9 with a half-life of 63.2 hours and 73.6 minutes, respectively (EPA, 2019. Hydrolysis of DBNPA is expected to be the dominant path of environmental degradation. DBNPA degrades into several compounds: dibromoacetonitrile (DBAN), dibromoacetamide (DBAM), dibromoacetic acid (DBAA), and 2-cyanoacetamine (CAM) (EPA, 2019 and PubChem).

DBNPA is also susceptible to photolysis. The substance degraded with half-lives of 14.8, 6.9, and 0.4 hours in the pH 5, pH 7, and pH 9 exposed test solutions, respectively (EPA, 2019). <1% of initial DBNPA remained after exposure to sunlight for 28 days (PubChem).

C. Biodegradation

The primary degradation pathway is through aerobic and anaerobic metabolism. In both anaerobic and aerobic metabolism studies, half-lives of less than 4 hours were measured for DBNPA; loss was due to both hydrolysis and biodegradation (EPA, 1994).

Low concentrations (0.6 mg/L and 0.06 mg/L) were used in an OECD 301B ready biodegradability study to account for the toxicity of DBNPA. At 0.06 mg/L DBNPA degraded with a half-life of 11-12 days and reached 72-77% degradation by 28 days, however this occurred outside of the 10-day window. At 0.6 mg/L, DBNPA exhibited less than 11% degradation by study termination (day 28). This is most likely due to the toxic nature of DBNPA inhibiting microorganisms in the sludge (EPA, 2019) [Kl. Score = 1]. Likewise, in an MITI test, there was 0% degradation of DBNPA, present at 100 mg/L, after 28 days; thus, DBNPA was not readily biodegradable in this test (PubChem).

DBNPA will rapidly degrade in aqueous aerobic and anaerobic environments forming two major (> 10%) degradates: DBAA and CAM. Half-lives were less than five hours (EPA, 2019).

While the rate of biodegradation in these tests does not satisfy the OECD criterion for readily biodegradability (60% in a 10-day window), the results do show that DBNPA is biodegradable at more realistic environmental exposure concentrations. If a chemical is found to be inherently biodegradable or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

D. Environmental Distribution

No experimental values were found. Using KOCWIN in EPISuite™ v. 4.11 (EPA, 2016), the estimated K_{oc} value from a Kow value of 0.82 is 58 L/kg. If released to soil, based on this K_{oc} value, the substance is expected to have high mobility. If released to water, based on the K_{oc} value and its water solubility, DBNPA is not expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

There are no reliable bioaccumulation studies on DBNPA. DBNPA is not expected to bioaccumulate based on a log K_{ow} of 0.80 – 0.88 (PubChem).

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

DBNPA is acutely toxic by the oral and inhalation routes, but not by the dermal route. It is corrosive to the skin and eyes. DBNPA is a skin sensitiser. Inhalation exposure of an aerosol or mist can cause respiratory irritation. Repeated oral exposures in rats showed some evidence of kidney toxicity. There was no evidence of systemic toxicity following repeated dermal exposures. It is not genotoxic or carcinogenic. It is not expected to cause reproductive or developmental effects.

B. Acute Toxicity

Oral

The oral LD50 values in rats are 235 mg/kg for males and 178 mg/kg for females (EPA, 2019) [Kl. Score = 3]. In another study, the oral LD50 in rats was 375 mg/kg for males and 284 mg/kg for females (EPA, 1994) [Kl. Score = 1]. The oral LD50 is 118 mg/kg in guinea pigs and 118 mg/kg in rabbits (EPA, 1994) [Kl. Score = 3].

Inhalation

The 4-hour LC50 in rabbits is 320 mg/m^3 (EPA, 1994).

Dermal

The dermal LD50 in rabbits is >2,000 mg/kg; no deaths were reported at this dose level (EPA, 1994) [Kl. Score = 1].

C. Irritation

Application of 0.5 g to the skin of rabbits for four hours produced erythema and edema with exfoliation after five days (EPA, 1994) [Kl. Score = 2]. In the acute dermal toxicity study, encrustation and exfoliation of the skin were observed (EPA, 1994).

DBNPA is corrosive to the eyes of rabbits (EPA, 1994). It is considered to be a severe eye irritant (NICNAS, 2016).

D. Sensitisation

DBNPA was a weak dermal sensitiser when tested in guinea pig sensitisation tests (EPA, 1994).

E. Repeated Dose Toxicity

Oral

Rats were dosed by oral gavage with 0, 5, 13, or 30 mg/kg DBNPA for 90 days. At >13 mg/kg, dyspnoea was seen in the treated animals, as well as weight loss and some deaths. The NOAEL for this study is 5 mg/kg/day (EPA, 1994) [Kl. Score = 1].

Male and female SD Spartan rats were given in their drinking water at pH 4 or 8 0, 20, 100, or 500 ppm DBNPA for 90 days. DBNPA is unstable at pH 8 and the objective of the study was to investigate the effect of the breakdown products of DBNPA. Minimal cytoplasmic swelling and vacuolisation were seen in the kidneys of the 500 ppm females at pH 8. No other treatment-related effects were noted. The NOAEL is 100 ppm, which corresponded to a daily intake of 8 and 15.9 mg/kg-day in males and females, respectively (PubChem and NICNAS, 2016) [Kl. Score = 2].

Male and female CD-1 mice were given in their feed 0, 3, 10, 100, 300, 600, or 1,000 mg/kg-day DBNPA (nominal doses) for 90 days. The actual average daily intakes were: 0, 1.58, 4.4, 44, 133, 267, or 447 mg/kg-day for males; and 0, 1.57, 4.5, 45, 137, 269, or 450 mg/kg-day for females. Decreased food consumption and body weight gain were noted in the >600 mg/kg males and >300 mg/kg females. Haemoglobin concentration and haematocrit were decreased in the 1,000 mg/kg males; red blood cell counts were decreased in the >300 mg/kg males, and serum chloride was increased in the >600 mg/kg males and >300 mg/kg females. Relative liver and spleen weights were increased and absolute brain and testes weights were decreased in the 1,000 mg/kg males, and heart weights were decreased in the 1,000 mg/kg females. Histopathologic examination showed no treatment-related effects. The NOAEL was reported to be 100 mg/kg-day (PubChem) [Kl. Score = 1].

Male and female F344 rats were given in their feed 0, 3, 10, 100, 300, 600, or 1,000 mg/kg-day DBNPA (nominal doses) for 90 days. The actual average daily intakes were: 0, 1.22, 4.6, 45, 133, 254, or 388 mg/kg-day for males; and 0, 1, 1.17, 4.3, 44, 130, 251, or 392 mg/kg-day for females. The discrepancy between nominal doses and the actual test material uptake was due to the poor stability of the test material in the dietary preparations despite the diets being prepared weekly. The 1,000 mg/kg males were euthanised on day 38 and the 600 mg/kg males and the 1,000 mg/kg females were euthanised on day 73. These groups were terminated prior to the end of the study because of minimal body weight gain and a concern that a large number of the animals would not survive to the end of the 90-day treatment period. At the end of 90 days, the mean body weights of the 300 mg/kg males and the 600 mg/kg females were significantly lower than controls. There was a significant decrease in the mean red blood cell count for the 300 mg/kg males and the mean haemoglobin concentration in the 100 and 300 mg/kg males were increased. Serum chloride levels were increased in the >100 mg/kg animals (both sexes), as well as a dose-related increase in urinary ketone content. Organ weight changes included: heart, kidney liver, brain, testes and epididymites, spleen, adrenal glands, ovaries, thymus, and uterus. Histopathologic examination showed possible adverse effects, such as axonal degeneration in the optic chiasma, optic nerve, and retinal atrophy in the eye. Specifically, the effects were: very slight vacuolisation in the cortex of the adrenal gland (100 and 300 mg/kg males); very slight or slightly diffuse hyperplasia of erythroid cells in the bone marrow (300 mg/kg males and 600 mg/kg females); focal or multifocal axonal degeneration optic

chiasma in the brain (300 mg/kg males) and in conjunction with this lesion slight or moderate unilateral axonal degeneration of the optic nerve and moderate unilateral retinal atrophy in the eye (300 mg/kg males); increased incidence of very slight or slight multifocal unilateral axonal degeneration of the optic nerve (600 mg/kg females); unilateral or bilateral multifocal degeneration of the seminiferous tubules in the testes (300 mg/kg males); slight atrophy of the cervix and ovaries (600 mg/kg females); and very slight atrophy of the thymal cortex (600 mg/kg females). The NOAEL was reported to be 10 mg/kg-day (4.6 and 4.3 mg/kg-day for males and females, respectively) based on the incidence of vacuolisation in the adrenal gland of the 100 mg/kg males and increased incidence of extramedullary haematopoiesis in the spleen and increased absolute spleen weights in the 100 mg/kg females (PubChem) [Kl. Score = 1].

Inhalation

A two-week inhalation toxicity study was conducted in rats. During the study, rats were exposed to 0, 0.51, 5.37 mg/m^3. A NOAEC of 0.5 mg/m^3 was established based on adverse histopathologic findings in the respiratory tract (diffuse hyperplasia of the respiratory epithelium, multifocal squamous metaplasia of the respiratory epithelium, multifocal inflammation of the lamina propria, multifocal necrosis of the respiratory epithelium, multifocal fibrosis), specifically the larynx (EPA, 2019).

Dermal

Male and female rats received dermal applications of 0, 103, 309, or 1,031 mg/kg DBNPA 6 hours/day, 5 days/week for 90 days. At 1,031 mg/kg, triglyceride levels were lower in males than controls; in females, cholesterol levels were lower, and serum alkaline phosphatase levels were higher than controls. The urinary pH was > in some males. Dermal irritation was transient in several male and female rats at >309 mg/kg. The NOAEL for systemic toxicity in this study is 309 mg/kg-day (EPA, 1994) [Kl. Score = 1].

F. Genotoxicity

In Vitro Studies

DBNPA was not mutagenic to *S. typhimurium* strains TA98, TA100, TA1535, TA1537, and TA1538 in the absence or presence of metabolic activation (EPA, 1994). DBNPA was not mutagenic to CHO cells in an HGPRT assay with or without metabolic activation (EPA, 1994). A weak positive response was seen in an in vitro chromosomal aberration test using human lymphocytes (EPA, 1994). Two separate in vitro unscheduled DNA synthesis (UDS) test using rat hepatocytes were negative (EPA, 1994).

In Vivo Studies

A negative result was reported for an *in vivo* micronucleus test in mice bone marrow (NICNAS, 2016).

No other adequate studies were located.

G. Carcinogenicity

No adequate studies on DBNPA were located.

As discussed in the RED, the hydrolysis of DBNPA produces, as the major degradate, DBAN which then degrades to DBAA, the rate of degradation is controlled by the pH. DBAA has been shown to cause increased incidence of degeneration of the liver in male rats, increased incidence of alveolar epithelial hyperplasia and nephropathy in female rats, and increased incidences of splenic hematopoiesis in male mice (Melnick *et al.,* 2007). Studies performed in rats, showed that DBAN causes effects in the GI tract. An NTP study performed in rats and mice, showed that rats developed squamous cell adenomas or carcinomas of the mouth. Two male rats had rare adenomas of the glandular stomach and male and female mice had increased rates of squamous cell papillomas of the forestomach. The NTP report also showed that there was a slight increase in the occurrence of liver tumours in male mice (NTP, 2010). Although the significance of these studies has not been evaluated by the Agency, they suggest that the degradation products of the parent compound (DBNPA) may cause cancer.

H. Reproductive/ Developmental Toxicity

DBNPA does not induce reproductive effects in dams or in offspring and does not induce any embryo or foetal toxicity or teratogenicity. Aspiration/gavage-related reflux of the chemical caused noisy and laboured respiration in rats and deaths in two dams treated with 30 mg/kg/day of DBNPA in a prenatal developmental toxicity study (EPA, 2019). Other effects observed at necropsy at 30 mg/kg/day were multifocal lung congestion, gaseous distension of the GI tract, and generalised mottled appearance of the lung. Similar effects were observed in two studies conducted via gavage: (i) a dose range-finding study performed in rats and (ii) a two-generation reproductive toxicity study performed in rats. For example, males and females of the F0 generation showed increased incidence of spongy/congested lungs, and F0 and F1 parental generations showed increased incidences of neurotoxic effects, distended gas filled stomach and intestines, dyspnoea and increased mortality. Based on these findings, a developmental and reproductive NOAEL of 30 mg/kg/day was established. Maternal or paternal NOAELs were lower at 10 mg/kg/day and 15 mg/kg/day, respectively (EPA, 2019) [Kl. Score =1].

I. Derivation of Toxicological Reference and Drinking Water Guidance Values

Toxicological reference values were derived for DBNPA following the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

The lowest NOAEL is from a 90-day oral gavage study that reported mortality, weight loss, and dyspnoea in rats dosed with 13 and 30 mg/kg-day DBNPA. The NOAEL for this study is 5 mg/kg-day (EPA 1994). The NOAEL from this study will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10

UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 10
UF_D (database uncertainty) = 1

Oral RfD = 5/(10 x 10 x 1 x 10 x 1) = 5/1000 = 0.005 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (0.005 x 70 x 0.1)/2 = 0.02 mg/L

Cancer

There were no studies on carcinogenicity conducted on DBNPA. Thus, a cancer reference value was not derived.

J. Human Health Hazard Assessment of Physico-Chemical Properties

DBNPA does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

DBNPA is very toxic to aquatic organisms. DBNPA is also moderately acutely toxic to birds.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of the acute aquatic toxicity studies conducted on DBNPA.

Table 3: Acute Aquatic Toxicity Studies on DBNPA

Test Species	% Active Ingredient (a.i.)	Endpoint	Results (mg/L)	Klimisch Score	Reference
Bluegill sunfish *(Lepomis macrochirus*)	100	96-hr LC_{50}	2.3	3	EPA, 2019
Bluegill sunfish *(Lepomis macrochirus*)	100	96-hr LC_{50}	1.3	-	EPA, 2019
Rainbow Trout (*Onchorhynchus mykiss)*	100	96-hr LC_{50}	1.0	-	EPA, 2019
Rainbow Trout (*Onchorhynchus mykiss)*	100	96-hr LC_{50}	2.3	3	EPA, 2019
Fathead minnow (*Pimephales promelas*)	99.1	96-hr LC_{50}	1.8	3	EPA, 2019
Fathead minnow (*Pimephales promelas*)	Degradate (96% DBAN)	96-hr LC_{50}	0.55	-	EPA, 2019
Sheepshead minnow (*Cyprinodon variegatus*)	99.5	96-hr LC_{50}	3.3	-	EPA,2019
Sheepshead minnow (*Cyprinodon variegatus*)	95	96-hr LC_{50}	1.71	-	EPA, 2019
Daphnia magna	95	48-hr EC_{50}	0.9	3	EPA, 2019
Daphnia magna	100	48-hr EC_{50}	0.86	3	EPA, 2019
Green algae *(Pseudokirchneriella subcapitata)*	99.87	96-hr EC_{50}	0.116		EPA, 2019

Chronic Studies

Table 4 lists the results of the chronic aquatic toxicity studies conducted on DBNPA.

Table 4: Chronic Aquatic Toxicity Studies on DBNPA

Test Species	% Active Ingredient (a.i.)	Endpoint	Results (mg/L)	Klimisch Score	Reference
Rainbow Trout (*Onchorhynchus mykiss)*	98	85-d NOEC	0.47	2	EPA, 2019
Daphnia magna	100	28-d NOEC	0.05	3	EPA, 2019
Green algae (*Pseudokirchneriella subcapitata)*	99.87	NOEC	0.058		EPA, 2019

C. Terrestrial Toxicity

Tables 5 and 6 lists the results of the chronic aquatic toxicity studies conducted on DBNPA.

Table 5: Terrestrial Acute Toxicity Studies on DBNPA

Test Species	% Active Ingredient (a.i.)	Results (mg/kg-bw)	Reference
Mallard Duck (*Anas platyrhynchos*)	Technical grade	205	EPA, 2019
Northern Bobwhite (*Colinus virginianus*)	Technical grade	150	EPA, 2019
Northern Bobwhite (*Colinus virginianus*)	100	354	EPA, 2019

Table 6: Terrestrial Subacute Toxicity Studies on DBNPA

Test Species	% Active Ingredient (a.i.)	Results (ppm)	Reference
Mallard Duck (*Anas platyrhynchos*)	95	>10,000	EPA, 2019
Mallard Duck (*Anas platyrhynchos*)	100	>5,620	EPA, 2019
Northern Bobwhite (*Colinus virginianus*)	95	>10,000	EPA, 2019
Northern Bobwhite (*Colinus virginianus*)	100	>5,620	EPA, 2019

D. Calculation of PNEC

The PNEC calculations for DBNPA follow the methodology discussed in DEWHA (2009).

PNEC water

Experimental results are available for three trophic levels. Acute E(L)C_{50} values are available for fish (1 mg/L), invertebrates (0.86 mg/L) and algae (0.116 mg/L). Results from chronic studies are also available for three trophic levels, with the lowest NOEC being 0.05 mg/L for invertebrates. On the basis that the data consists of short-term and long-term results from three trophic levels, an assessment factor of 50 has been applied to the lowest reported NOEC of 0.05 mg/L for invertebrates. The $PNEC_{water}$ is 0.001 mg/L.

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Moreover, the substance is not expected to substantially partition to sediments. Nonetheless, a $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 0.0015 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= 1.91/1280 \times 1000 \times 0.001$
$= 0.0015$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3[default]
$PNEC_{water}$ = 0.001 mg/L

$K_{sed\text{-}water} = 0.8 + [(0.2 \times Kp_{sed})/1000 \times BD_{solid}]$
$= 0.8 + [(0.2 \times 2.32)/1000 \times 2400]$
$= 1.91\ m^3/m^3$

And:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3[default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 58 \times 0.04$
$=2.32$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). Using KOCWIN in EPISuite™ v. 4.11 (EPA, 2016), the estimated K_{oc} value from a K_{ow} value of 0.82 is 58 L/kg.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 0.00077 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (1.16/1500) \times 1000 \times 0.001$
$= 0.00077$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 kg/m^3 [default]

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 58 \times 0.02$
$= 1.16\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). Using KOCWIN in EPISuite™ v. 4.11 (EPA, 2016), the estimated K_{oc} value from a K_{ow} value of 0.82 is 58 L/kg.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

DBNPA is biodegradable at expected environmental exposure concentrations. Thus, DBNPA does not meet the screening criteria for persistence.

Based on an experimental log K_{ow} value is 0.8, DBNPA does not meet the screening criteria for bioaccumulation.

The lowest chronic NOEC for DBNPA is <0.1 mg/L. Thus, DBNPA meets the screening criteria for toxicity.

The overall conclusion is that the DBNPA is not a PBT substance.

B. Other Characteristics of Concern

Only tier 3 chemicals which trigger persistence and bioacummulative thresholds are considered to be chemicals with a potential for cumulative impacts. As noted in the prior section, DBNPA does not meet the criteria for persistence or bioaccumulation.

No other characteristics of concern were identified for DBNPA.

9 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
2,2-dibromo-3-nitrilopropionamide	10222-01-2	Not a PBT	No	No	No	No	No	Yes	3	3	3

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 - Tier 3 - Quantitative Risk Assessment: Complete PBT, qualitative and quantitative assessment of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
GHS	Globally Harmonised System of Classification and Labelling of Chemicals
IUPAC	International Union of Pure and Applied Chemistry
kg	kilograms
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mg/m^3	milligrams per cubic metre
mL	millilitre
mPa s	millipascal second

MW	molecular weight
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEC	No Observed Adverse Effect Concentration
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency