

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 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).

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 rationale 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)	<i>Selenastrum capricornutum</i>	0.09	10	0.009

EC₅₀ = 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

EC₅₀ = 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

EC₅₀ = 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., C₁₂) or as a mixture of different chain lengths (e.g., C₁₂ to C₁₈). The most common AO in commerce is the alkyl dimethyl AO, where the alkyl group contains 10 to 16 carbon atoms, predominately C₁₂ and C₁₄, and the average chain length is C_{12.9}.

The molecular structure for a C₁₂ dimethyl amine oxide, is presented in **Figure 1**.

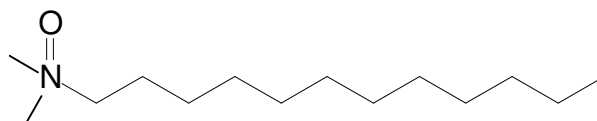


Figure 1 Molecular Structure of C₁₂ dimethyl amine oxide ²

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 alkyl dimethyl, 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, ophthalmoscopic 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). Estimated concentrations in treated water (refer **Attachment 2**) are less than the derived drinking water guideline value of 1.5 mg/L.

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*.

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, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia. Available: <https://www.nepc.gov.au/sites/default/files/2022-09/cmgt-nchem-eragm-industrial-chemicals-200902.pdf>
- frc environmental. 2021. Santos GLNG Dawson River Watercourse Releases: Receiving Environment Monitoring Program. April 2021.
- OECD (2006). OECD-SIDS Initial Assessment Report and Dossiers for Amine Oxides. Available at: https://hpcvchemicals.oecd.org/UI/SIDS_Details.aspx?id=B927B43D-8E91-4ADA-80E3-720D634E01C0.



Santos, 2013. Dawson River Release Scheme – Environmental Authority Amendment Application – Supporting Information. May 2013.



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 sensitizer. 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 alkyl dimethylamine oxides

CAS RN: 61788-90-7

Molecular formula: $\text{CH}_3(\text{CH}_2)_R\text{N}(\text{CH}_3)_2\text{O}$ where R is 9-17 (UVCB substance)

Molecular weight: Unspecified (UVCB substance)

Synonyms: Cocamine oxide; coco dimethylamine oxide; coconut dimethylamine oxide; N-(cocoalkyl)-dimethylamine oxide; N,N-dimethylcocamine 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 sensitizer. 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 CO₂. 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 LD₅₀ 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 LD₅₀ in rats of amine oxides, cocoalkyldimethyl was 3,873 mg/kg (OECD, 2006) [Kl. score = 2].

Inhalation

No inhalation studies available.

Dermal

The dermal LD₅₀ 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 sensitizer 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 $\geq 0.2\%$ females. The ophthalmoscopic examination showed lenticular opacities in the posterior cortex of the $\geq 0.2\%$ 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 alkyl dimethyl, 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 ophthalmoscopic 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 alkyl dimethyl, 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, ophthalmoscopic 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 alkyl dimethyl, 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, cocoalkyl dimethyl 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 (<i>S. typhimurium</i> 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 F₁ 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 F₁ animals were similar between treated and control groups; F₁ females from the 200 mg/kg F₀ group had slightly elevated fetal and placental weights. There were no macroscopic changes seen in the F₁ 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 ≥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)

$$\text{Oral RfD} = \text{NOAEL} / (\text{UF}_A \times \text{UF}_H \times \text{UF}_L \times \text{UF}_{\text{Sub}} \times \text{UF}_D)$$

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

$$\text{Oral RfD} = 42 / (10 \times 10 \times 1 \times 1 \times 1) = 42 / 100 = \underline{0.4 \text{ mg/kg-day}}$$

Drinking water guidance value

$$\text{Drinking water guidance value} = (\text{animal dose}) \times (\text{human weight}) \times (\text{proportion of intake from water}) / (\text{volume of water consumed}) \times (\text{safety factor})$$

Using the oral RfD,

$$\text{Drinking water guidance value} = (\text{oral RfD}) \times (\text{human weight}) \times (\text{proportion of water consumed}) / (\text{volume of water consumed})$$

where:

Human weight = 70 kg (ADWG, 2011)

Proportion of water consumed = 10% (ADWG, 2011)

Volume of water consumed = 2L (ADWG, 2011)

$$\text{Drinking water guidance value} = (0.42 \times 70 \times 0.1) / 2 = \underline{1.5 \text{ mg/L}}$$

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
<i>Salmo gairdneri</i>	96-hr LC ₅₀	13	1	OECD, 2006
<i>Brachydanio rerio</i>	96-hr LC ₅₀	1.0	2	OECD, 2006
<i>Leuciscus idus melanotus</i>	96-hr LC ₅₀	4.3	2	OECD, 2006
<i>Daphnia magna</i>	48-hr EC ₅₀	2.9	1	OECD, 2006
<i>Selenastrum capricornutum</i>	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 EC₂₀ 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:

$$\begin{aligned} \text{PNEC}_{\text{sed}} &= (K_{\text{sed-water}}/\text{BD}_{\text{sed}}) \times 1000 \times \text{PNEC}_{\text{water}} \\ &= 30.08/1280 \times 1000 \times 0.009 \\ &= 0.2115 \text{ mg/kg} \end{aligned}$$

Where:

$K_{\text{sed-water}}$ = suspended matter-water partition coefficient (m^3/m^3)

BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 kg/m^3 [default]

$\text{PNEC}_{\text{water}}$ = 0.009 mg/L

$$\begin{aligned} K_{\text{sed-water}} &= 0.8 + [(0.2 \times K_{\text{p}_{\text{sed}}})/1000 \times \text{BD}_{\text{solid}}] \\ &= 0.8 + [(0.2 \times 61)/1000 \times 2400] \\ &= 30.08 \text{ m}^3/\text{m}^3 \end{aligned}$$

And:

$K_{\text{p}_{\text{sed}}}$ = solid-water partition coefficient (L/kg)

BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 kg/m^3 [default]

$$\begin{aligned} K_{\text{p}_{\text{sed}}} &= K_{\text{oc}} \times f_{\text{oc}} \\ &= 1525 \times 0.04 \\ &= 61 \text{ L/kg} \end{aligned}$$

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:

$$\begin{aligned} \text{PNEC}_{\text{soil}} &= (\text{Kp}_{\text{soil}}/\text{BD}_{\text{soil}}) \times 1000 \times \text{PNEC}_{\text{water}} \\ &= (30.5/1500) \times 1000 \times 0.009 \\ &= 0.18 \text{ mg/kg dw} \end{aligned}$$

Where:

Kp_{soil} = soil-water partition coefficient (m³/m³)

BD_{soil} = bulk density of soil (kg/m³) = 1,500 kg/m³ [default]

$$\begin{aligned} \text{Kp}_{\text{soil}} &= \text{K}_{\text{oc}} \times \text{f}_{\text{oc}} \\ &= 1525 \times 0.02 \\ &= 30.5 \text{ m}^3/\text{m}^3 \end{aligned}$$

Where:

K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for amine oxides, cocoalkyldimethyl 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 (IChEMS, 2022; 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
IChEMS	Industrial Chemicals Environmental Management Standard
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