

Santos

GLNG Project

APPENDIX G ENVIRONMENTAL ASSESSMENT PROFILES

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G.1 SCHLUMBERGER GUAR BASED SYSTEMS

Environmental Assessment

Ammonium C6-C10 Alcohol Ethoxysulfate (CAS No. 68187-17-7)

Alcohol ethoxysulfates (AES) are a widely used class of anionic surfactants. No data could be located on alcohol ethoxysulfates in the C6 to C10 range.

In the HERA report, the alcohol ethoxysulfate family covers commercial grades of linear-type primary alcohol ethoxysulfates of either sodium, ammonium or triethanolamine (TEA) salts. Sodium salts of AES are by far the commonly used grades.

In the absence of data, the C12-C14 alcohol ethoxysulfates were used as read-across to the C6-C10 alcohol ethoxysulfates.

Biodegradation

AES are readily biodegradable under aerobic conditions, with alkyl-chain length having little effect. AES are expected to be easily biodegradable under anaerobic conditions based on the biodegradation data on alcohol ethoxylates and alkyl sulfates. In a stringent anaerobic biodegradability test (ECETOC test) on C12-14EO2S, gas (CO₂ and methane) production of 75% occurred within the 41-day incubation period.

Surface-water degradation rate of 0.48 per day has been applied to all chain lengths based on measured data for C14-15EO2.25S.

Biodegradation Pathways

The risk assessment of a parent compound should be restricted to that compound unless the metabolites are persistent and/or more ecotoxic than the parent. There are three starting routes of AES degradation which all seem to occur: i) ω - β -oxidation of the alkyl chain, ii) enzymatic cleavage of the sulfate substituent leaving an alcohol ethoxylate, iii) cleavage of an ether bond in the AES molecule producing either the alcohol (central cleavage) or an alcohol ethoxylate and an oligo (ethylene glycol) sulfate. The subsequent degradation of the resulting intermediates encompasses oxidation of the alcohol to the corresponding fatty acid (itself then degraded via β -oxidation) or degradation of the alcohol ethoxylate (via central cleavage or degradation from either end of the molecule) or degradation of the oligo (ethylene glycol) sulfate. The ultimate biodegradability of alcohol ethoxylates is well established and glycol ether sulfates have also been shown to be fully degradable by mixed cultures forming inorganic sulfate and carbon dioxide. The conclusion that AES degradation will not produce any recalcitrant metabolite is in line with the experimental findings on AES in the "Test for Detecting Recalcitrant Metabolites" (Gerike and Jasiak, 1986). In addition, Yoshimura and Matsuda (1982) reported test data showing that the (fish) toxicity of AES decreases in the course of AES

degradation. Consequently, there is no indication for the formation of persistent or markedly toxic metabolites from AES.

Aquatic Toxicity

Acute toxicity data are available in several review articles. As a large chronic data base exists the acute data have not been further considered for the HERA risk assessment. The abundance of chronic toxicity data is such that it is justified to base the PNEC on chronic toxicity data.

Determination of PNECs

PNEC_{aquatic}: The chronic toxicity QSAR (Dyer *et al.*, 2000) has been used to derive PNEC values, using an assessment factor of 10. The assessment factor of 10 is justified by the taxonomic diversity of the overall dataset. The resulting PNEC are shown in the table below.

PNEC_{aquatic} (mg/L)

Carbon #	12	13	14
PNEC _{aquatic} (mg/L)	0.27	0.076	0.038

A PNEC_{aquatic} value of 0.27 mg/L was used for C6-C10 alcohol ethoxysulfates based on the value for C12 alcohol ethoxysulfates.

PNEC_{sediment}: There are no measured sediment exposure data nor any sediment toxicity data on AES. Since the log Kow of none of the AES homologues exceeds log Kow 5, the TGD states that the risk characterization for the aquatic compartment should be used for the sediment compartment. Consequently PNEC_{sediment} was not calculated in the HERA report.

PNEC_{soil}: To estimate PNEC_{soil} by equilibrium partitioning, the sorption behavior of AES homologues is needed. The only sorption value found for AES was measured for C₁₂EO₅S in river sediments and gave K_{oc}=1.1 (Urano *et al.*, 1984). This compares to a K_{oc} of 2.3 calculated using the QSAR for 'Predominantly hydrophobics' from Sabljic & Gusten (1995) referenced in the TGD (log K_{oc}=0.81 log Kow + 0.1). The applicability of this QSAR to surfactants is questionable, but in the absence of other measured K_{oc} values, PNEC_{soil} have been derived using this QSAR. Using a K_{oc} of 2.3 and a PNEC_{aquatic} of 0.27 mg/L, the PNEC_{soil} was calculated to be 0.0083 mg/kg.

References

Dyer, S.D., Stanton, D.T., Lauth, J.R. and Cherry, D.S. (2000). Structure-activity relationships for acute and chronic toxicity of alcohol ether sulfates. *Environmental Toxicology and Chemistry* 19: 608-616.

Gerike P., and Jasiak, W. (1986). How completely are surfactants biodegraded? *Tenside Deterg.* 23: 300-304.

Human and Environmental Risk Assessment (HERA) on Ingredients of Household Cleaning Products: Alcohol Ethoxysulphates, Human Risk Assessment (2003), Draft <http://www.heraproject.com>

Sabljić, A., and Güsten, H. (1995). QSARs for soil sorption. In: Overview of structure-activity relationships for environmental endpoints. Hermens JLM (ed), Report prepared within the framework of the project 'QSAR for Prediction of Fate and Effects of Chemicals in the Environment', an international project of the Environmental Technologies RTD Programme (DG XII/D-1) of the European Commission under contract number EV5V-CE92-0211.

Urano, K, and Saito, M. (1985). Biodegradability of surfactants and inhibition of surfactants to biodegradation of other pollutants. *Chemosphere* 14: 1333-1342.

Yoshimura, K., and Masuda, F. (1982). Biodegradation of Sodium Alkyl Poly(oxyalkylene)sulfates *J. Am. Oil Chem. Soc.* 59: 328-332.

Environmental Assessment

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Sabljić, A., and Güsten, H. (1995). QSARs for soil sorption. In: Overview of structure-activity relationships for environmental endpoints. Hermens JLM (ed), Report prepared within the framework of the project 'QSAR for Prediction of Fate and Effects of Chemicals in the Environment', an international project of the Environmental Technologies RTD Programme (DG XII/D-1) of the European Commission under contract number EV5V-CE92-0211.

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Yoshimura, K., and Masuda, F. (1982). Biodegradation of Sodium Alkyl Poly(oxyalkylene)sulfates *J. Am. Oil Chem. Soc.* 59: 328-332.

Environmental Assessment

Amorphous/Non-crystalline Silica (CAS No. 7631-86-9¹)

Silica Gel (CAS No. 112926-00-8)

Amorphous Silica and silica gel have been reviewed in the OECD-SIDS program (OECD, 2004a,b).

The CAS No. 7631-86-9 is the general CAS registry number for silicon dioxide which includes all forms of silicas (*e.g.*, also crystalline and natural forms). Only the silica subclasses, the synthetic amorphous silicas, are subject of this assessment.

Synthetic amorphous silica and silicates are in powder form which have a low water solubility, based on the sum of soluble SiO₂ and cations (water-soluble fraction): ≤70 mg/l (SAS), approx. 70 – 80 mg/l (NAS), and approx. 260 mg/l (CS) at 20 °C.

Environmental Fate and Transport

Silicon oxides are the most abundant compounds in the earth's crust mass. 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 vapor pressure.

Synthetic amorphous silica and silicates released into the environment are expected to combine indistinguishably with the soil or sediment due to their similarity with inorganic soil/sediment matter and will be subjected to natural processes under environmental conditions (cation exchange, dissolution, sedimentation).

Biodegradation is not applicable to these inorganic substances. The bioavailable form of synthetic amorphous silica and silicates is the dissolved form which exists exclusively as monosilicic [Si(OH)₄] acid under environmental pH. In analogy to the general chemical reaction of weak acids and salts of weak acids with water, the water-soluble fraction of silica acts as a weak acid and, therefore, will tend to lower the pH value, while that of a silicate acts as a base tending to bind protons and, thus, raise the pH value by forming hydroxyl ions. But pH shifts which are measurable at high loadings under laboratory conditions are not expected to occur from the anthropogenic deposition in the aquatic environment of synthetic amorphous silicas due to low aquatic releases and sufficient natural buffer capacities. Finally, these materials are supposed to combine indistinguishably with the soil layer or sediment due to their chemical similarity with inorganic soil matter.

Dissolved silica can be actively assimilated by some marine and terrestrial organisms as normal natural processes mainly related to structural function.

Aquatic Toxicity

Studies on fish, Daphnia and algae using excess loadings of SAS or NAS showed no acute toxicity, although physical effects on Daphnia were observed in tests using unfiltered test medium. Test results, based on loading rates, are as follows: 96-hour LL₀ (*Brachydanio rerio*) is 10,000 mg/L for SAS and NAS; 24-hour EL₅₀ (*Daphnia magna*) >10,000 mg/L for SAS; 72-hour NOEL (*Scenedesmus subspicatus*) is 10,000 mg/L for NAS.

There are no chronic aquatic toxicity data, but due to the known inherent physico-chemical properties, absence of acute toxic effects as well as the ubiquitous presence of silica/silicates in the environment, there is no evidence of harmful long-term effects arising from exposure to synthetic amorphous silica/silicates.

Toxicity to Terrestrial Organisms

No data are available.

PBT Assessment

Noncrystalline silica (silica gel) is silicon dioxide, an inorganic compound which is ubiquitous in the environment. For the purposes of this PBT assessment, the persistent criteria is not considered applicable to this inorganic salt.

A log K_{ow} is not applicable to noncrystalline silica. Noncrystalline silica (silica gel), as a stable crystalline solid, is expected to have negligible uptake through the gill or gut of aquatic organisms. Thus, noncrystalline silica (silica gel) is not expected to bioaccumulate.

No chronic toxicity data exist on noncrystalline silica or silica gel; however, the acute EC(L)₅₀s are >0.1 mg/L in fish, invertebrates and algae. Thus, noncrystalline silica (silica gel) does not meet the screening criteria for toxicity.

The overall conclusion is that noncrystalline silica (silica gel) is not a PBT substance.

References

OECD (2004a). IUCLID Data Set for Synthetic Amorphous Silica and Silicates: Silicon Dioxide (CAS No. 7631-86-9, 112945-52-5, 112926-00-8; Silicic Acid, Aluminum Sodium Salt (CAS No. 1344-00-9); Silicic Acid, Calcium Salt (CAS No. 1344-95-2), UNEP Publications.

OECD (2004b). Screening Information Dataset (SIDS) Initial Assessment Report for Synthetic Amorphous Silica and Silicates: Silicon Dioxide (CAS No. 7631-86-9, 112945-52-5, 112926-00-8; Silicic Acid, Aluminum Sodium Salt (CAS No. 1344-00-9); Silicic Acid, Calcium Salt (CAS No. 1344-95-2), UNEP Publications.

Environmental Assessment

C6-C10 Alcohol Ethoxylates

The alcohol ethoxylate (AE) family is defined for the HERA report purposes to be of the basic structure C_x-yAEn. The subscript following the 'C' indicates the range of carbon chain units. AEs with carbon unit range between C8 to C18 are most commonly used in household detergent products. Further, AEs contain an ethylene oxide (E) chain attached to the alcohol. The degree of ethylene oxide polymerization is indicated by a subscript which indicates the average number of ethylene oxide units. In household products the average ethylene oxide chain length commonly ranges between 3 and 12 units.

Biodegradation

AE homologues with hydrocarbon chain lengths ranging from 8 to 18 and with from 2 to more than 20 ethylene oxide units are readily biodegradable.

As a class, AE undergo rapid primary and ultimate biodegradation under both laboratory and field conditions. The biodegradability of the different AE homologues used in HERA applications is relatively unaffected by the alkyl carbon chain length and the number of EO units.

Proposed half-lives in river water at 12°C: 4 to 24 hours (based on experimental data).

AE are also anaerobically biodegradable.

Bioaccumulation

The AE homologues used for domestic cleaning applications are very likely to have a log K_{ow} value greater than 3.

Environment Canada and Health Canada (2006) has established that the degree of bioaccumulation expected from AE is well below the Canadian bioconcentration criterion of 5000. The sixteen measured BCF values for 15 AE homologues showed the lack of a linear relationship between alkyl or ethoxylate chain length and BCF, with the highest measured BCF value being under 800. Environment Canada (2006) concluded that it is evident that the AE metabolism rates prevent any significant accumulation. The data indicated that there may be an optimal structural combination of ethoxylate and alkyl chain lengths, at or around C14EO7, where BCF is maximized, but even the measured BCF for this chemical is well below the criterion of 5000. Thus Environment Canada (2006) concluded that ethoxylated aliphatic alcohols are not bioaccumulative.

Aquatic Toxicity

Acute aquatic effects data are presented in the HERA report to only establish that the essentially linear and branched AE used in household detergents are not more toxic than the linear AE which have the same uses. The toxicity mechanism for AE is accepted to be non-polar narcosis, in which the AE homologues with longer hydrocarbon chains and higher log K_{ow} are more efficient at penetration of the cell membrane, and thus more toxic. However, the AE homologues must be sufficiently soluble in water to allow a toxic concentration to reach the target organism. For the long chain alcohols, generally the least soluble and the most toxic of the AE homologues, the long chain alcohol OECD-Screening Information Assessment Report (SIAR) (SIAR, 2006) shows that the toxicity is restricted by solubility considerations at hydrocarbon chain lengths of 15 and above. Although the addition of ethylene oxide groups makes the other AE homologues more soluble, solubility considerations may reduce the toxicity of several higher hydrocarbon chain length and lower EO chain length AE. The available acute toxicity data follows this generally accepted pattern, and also indicates that the linear, essentially linear and branched AE are of similar toxicity.

Toxicity to Terrestrial Organisms

Acute soil toxicity measurements for both plants and soil invertebrates are available from standard tests carried out on commercial AE mixtures, which contain differing distributions of AE homologues. The available data are reviewed in the HERA report.

A range of chronic soil tests has been carried out for two pure AE homologues, C12EO4 and C16EO4. The two AE homologues chosen for the chronic tests span the hydrocarbon chain length range of high tonnage AE, and have an EO chain length value at which the toxicity is expected to be in the high range for each hydrocarbon chain length. The chronic tests, to assess the survival and reproduction of earthworms (*Eisenia fetida fetida*), springtails (*Folsomia candida*), and nematodes (*Caenorhabditis elegans*), were carried out using a natural sandy loam soil, with an organic carbon content of 1.3%, which could be assumed to be free of pesticide. If an application factor of 10 were applied to the lowest chronic NOEC value to determine a PNEC, a PNEC of 22 mg/kg would result for C12EO4 and a PNEC of 46 mg/kg would result for the C16EO4 AE homologue. Comparison of the acute test data with the equilibrium partition soil PNEC values show very similar values. Thus, the chronic soil toxicity results for C12EO4 and C16EO4 support the validity of the PNEC values determined by equilibrium partitioning.

Information showing the relatively small difference between acute and chronic toxicity for soil organisms means that available single homologue acute data also supports the PNEC calculated by equilibrium partitioning from aquatic monitoring data. In addition, available data for AE mixtures is consistent with the equilibrium partitioning PNEC values.

Determination of PNEC_{aquatic}

The chronic *Daphnia magna* QSAR developed by Boeije *et al.* (2006) can be used, with an appropriate application factor, to determine the PNEC for each AE homologue. Of the three trophic level QSARs discussed here, the chronic *Daphnia magna* QSAR is the most robust. The algal QSAR work by Wind and Belanger (2006) has shown that AE toxicity to algae, daphnia, and fish are of similar magnitude, while the chronic AE toxicity data given indicates that *Daphnia magna* are among the most sensitive invertebrates.

The PNEC values determined for each AE homologue using both the chronic *Daphnia magna* QSAR with an application factor of 10 given in Table 4.38 of the HERA report. For the *Daphnia magna* QSAR, the application factor of 10 is used as three chronic QSARs are available for AE homologues. The *Daphnia magna* QSAR has been chosen as it is the most robust of these three chronic QSARs, and has the most sensitive endpoint over much of the range of AE homologues.

The composition of C6-C10 alcohol ethoxylates are unknown. It is possible that it is a mixture of linear and branched alcohol ethoxylates with varying EO chain lengths. Therefore, a mean PNEC for this CASRN was calculated as follows: for each hydrocarbon chain length number, the PNEC value AE with EO units 1 to 20 were average together, providing a mean value that covers the range of PNECs for that hydrocarbon chain length number. Each of these mean PNECs were then averaged together to cover the hydrocarbon chain lengths included in this CASRN. It should be noted that the HERA document does not cover hydrocarbon numbers less than C8 and therefore PNEC values were not calculated for the C6 and C7 alcohol ethoxylates. Without knowing the hydrocarbon distribution in the supplier product, it is unclear how the limited data will influence the overall PNEC value for this substance.

PNEC_{aquatic}: Chronic *Daphnia magna* QSAR and an Application Factor of 10

	C8 + C9 (mg/L)	C10 (mg/L)
Mean	3.54	1.71
Range	0.171 – 11.9	0.118 – 6.23

$$\text{PNEC}_{\text{aquatic}} (\text{freshwater}) = (3.54 + 1.71)/2 = 2.63 \text{ mg/L}$$

Determination of PNEC_{sediment}

The equilibrium partitioning method is used to predict the sediment PNEC from the aquatic PNEC, if no sediment data are available. A probabilistic QSAR has been developed for aquatic species based on chronic data (see HERA report). This QSAR contains aquatic test data for species which live in sediment, such as *Chironomus tentans* and *Corbicula fluminea*, and others which live near or in the top sediment surface such as *Hyallolella azteca*, *Dugesia gonocephala*, *Chlorella vulgaris* and *Navicula pelliculosa*.

Comparison of the chronic *Daphnia magna* data (which was used to derive the aquatic PNEC) with that for the sediment dwelling organisms shows that *Daphnia magna* is of similar sensitivity to the sediment dwelling organisms. As the deterministic chronic *Daphnia magna* QSAR is quite robust, and for the purposes of consistency, it was decided that the aquatic PNEC derived from the chronic *Daphnia magna* QSAR be used with the equilibrium partitioning method to determine the PNEC sediment for all the AE homologues. A mean PNEC for this CASRN was calculated similar to the approach for PNEC_{aquatic}.

The HERA report used the TGD (2003) approach to calculate the PNEC sediment using the equilibrium partitioning method according to $PNEC_{sed} = (K_{susp-water} / R_{hosusp}) * PNEC_{water} * 1000$.

PNEC_{sediment} values determined by the equilibrium partitioning method, based on the deterministic method using the chronic *Daphnia magna* QSAR

	C8 + C9 (mg/kg)	C10 (mg/kg)
Mean	232	254
Range	2.76 - 1140	3.11 - 1250

$$PNEC_{sediment} = (232 + 254)/2 = 243 \text{ mg/kg}$$

Determination of PNEC_{soil}

The equilibrium partitioning calculation for PNEC_{soil} has been carried out using the PNEC_{aquatic} values determined by using the deterministic *Daphnia magna* QSAR with an application factor of 10. The results of this calculation are shown in Table 4.47 of the HERA report for each AE homologue. A mean PNEC for this CASRN was calculated similar to the approach for PNEC_{aquatic}.

PNEC_{soil} values determined by the equilibrium partitioning method, based on the deterministic method using the chronic *Daphnia magna* QSAR

	C8 + C9 (mg/kg)	C10 (mg/kg)
Mean	89	187
Range	1.03 - 440	2.14 - 1012

$$PNEC_{soil} = (89 + 187)/2 = 138 \text{ mg/kg}$$

References

Boeije, G. M., Cano, M. L., Marshall, S. J., Belanger, S. E., Van Compernelle, R. , Dorn, P. B., Dorn, Gumbel, H., Toy, R., Wind, T. (2006). Ecotoxicity QSARs for alcohol ethoxylates based on the mixture toxicity concept. *Ecotoxicol. Environ. Safety* 64: 75-84.

Environment Canada and Health Canada. (2006). Response to the ICG Aliphatic Working Group's Proposal Regarding Environment Canada' Preliminary Categorization of Ethoxylated Aliphatic Alcohols, p. 4, February 2006, Ottawa Canada.

Human and Environmental Risk Assessment (HERA) on Ingredients of Household Cleaning Products: Alcohol Ethoxylates (2009) <http://www.heraproject.com>

Van Compernelle, R., McAvoy, D., Sherren, A., Wind, T., Cano, M.L., Belanger, S.E., Dorn, P.B., and Kerr, K.M. (2006). Predicting the sorption of fatty alcohols and alcohol ethoxylates to effluent and receiving water solids. *Ecotoxicol. Environ. Safety* 64: 61–74.

Wind, T., and Belanger, S.E. (2006). Acute and chronic toxicity of alcohol ethoxylates to the green alga, *Desmodesmus subspicatus*, and structure-activity-relationships. *Bull. Environ. Contamin. Toxicol.* 76: 218-225.

Environmental Assessment

Crystalline Silica, Quartz (CAS No. 14808-60-7)

Crystalline Silica, Cristobalite (CAS No. 14464-46-1)

Silica is an off-white granule that occurs naturally in various crystalline and amorphous or other non-crystalline forms. Crystalline silica is characterized by silicon dioxide (SiO₂) 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.

Crystalline silica, quartz and crystalline silica, cristobalite are naturally occurring minerals that are insoluble in water.

They are persistent in the environment.

Crystalline silica, quartz, and crystalline silica, cristobalite as minerals, are not expected to bioaccumulate or be toxic to aquatic organisms because of their water insolubility and lack of bioavailability.

Crystalline silica, quartz and crystalline silica, cristobalite are not considered to be PBT substances.

Environmental Assessment

Diammonium peroxodisulfate Ammonium persulfate (CAS No. 7727-54-0)

Diammonium peroxisulfate or ammonium persulfate has been reviewed in the OECD-SIDS program (OECD, 2005a,b).

Environmental Fate

The inorganic persulfates are soluble in water (≥ 60 g/L) and their vapor pressures are negligible. Ammonium persulfate will be distributed into the water compartment in the ionic form of the ammonium cation and persulfate anion. Ammonium persulfate is expected to degrade in the environment mainly via hydrolysis, but metal catalyzed decomposition, and reactions with organic chemicals in the soil or water also are possible.

Persulfates are not expected to adsorb to soil due to its dissociation properties, instability (hydrolysis) and high water solubility. Persulfates should behave as free ions or decompose into sulfate ions. In soils, upon decomposition, the cation could form more stable sulfate or bisulfate salts.

Persulfates are not expected to bioaccumulate in the soil or in aqueous solution. They will decompose into inorganic sulfate or bisulfate.

Aquatic Toxicity

The 96-hour LC₅₀ values for ammonium persulfate to fish are from 76 to 323 mg/L. The acute toxicity EC₅₀ values for invertebrates are from 120 to 391 mg/L. The 72-hour EC₅₀ values for ammonium persulfate to algae are 83.7 mg/L.

Toxicity to Terrestrial Organisms

No data were available.

Determination of PNECs

PNEC_{aquatic}: Experimental results are available for three trophic levels. Acute E(L)C₅₀ values are available for fish (76 mg/L), Daphnia (120 mg/L), and algae (84 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 effect concentration of 76 mg/L for fish. The PNEC_{aquatic} is 0.076 mg/L.

PNEC_{sediment}: No experimental toxicity data on sediment organisms are available. Diammonium peroxodisulfate dissociates completely in water with its environmental distribution is dominated by its high water solubility. Kow and Koc do not readily apply to inorganics, such as diammonium peroxodisulfate. Thus, the equilibrium partitioning method cannot be used to calculate the PNEC_{sediment}. Based on the its properties, no adsorption of diammonium peroxodisulfate 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 terrestrial organisms are available. The environmental distribution of diammonium peroxodisulfate is dominated by its water solubility. Sorption of diammonium peroxodisulfate should probably be regarded as a reversible situation, *i.e.*, the substance is not tightly nor permanently bound. Kow and Koc parameters do not readily apply to inorganics, such as diammonium peroxodisulfate. Thus, the equilibrium partitioning method cannot be used to calculate the PNEC_{soil}. Based on the its properties, diammonium peroxodisulfate is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

References

OECD (2005a). 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.

OECD (2005b). Screening Information Dataset (SIDS) Initial Assessment Report for Ammonium persulfate (CAS No. 7727-54-0); Potassium persulfate (CAS No. 7727- 27-1); Sodium persulfate (CAS No. 7775-27-1), UNEP Publications.

Environmental Assessment

Diatomaceous Earth (CAS No. 61790-53-2)

Uncalcined diatomaceous earth (CAS No. 61790-53-2) typically contains around 1% crystalline silica. When diatomaceous earth is subjected to pressure or is processed ("calcined") at temperatures above 1000°C some of the amorphous silica is converted to crystalline silica in the form of cristobalite. Calcined diatomaceous earth can contain anywhere from 1% to 75% cristobalite.

Diatomaceous earth and crystalline silica are naturally occurring minerals that are insoluble in water.

They are persistent in the environment.

Diatomaceous earth and crystalline silica as minerals, are not expected to bioaccumulate or be toxic to aquatic organisms because of their water insolubility and lack of bioavailability.

Diatomaceous earth and crystalline silica, quartz are not considered to be PBT substances.

Environmental Assessment

Guar Gum (CAS No. 9000-30-0)

Guar gum (CAS No. 9000-30-0) is the milled endosperm of the leguminous plant *Cyanopsis tetragonolobus*. Structurally, it is a galactomannan (a polysaccharide) 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 -(1-4) linked, and the single D-galactose units are joined to the main chain by α -(1-6) linkages. The estimated molecular weight of guar gum ranges from 200,000 to 300,000 daltons (Glickman, 1969).

Biodegradation

No information was found. Guar gum, being a polysaccharide composed of galactomannan, would be expected to be readily biodegradable.

Bioaccumulation

Not expected to bioaccumulate as a polysaccharide composed of galactomannans.

Aquatic Toxicity

The 48-hour LC₅₀ for *Daphnia magna* was reported to be 42 mg/L (Biesinger *et al.*, 1976).

Toxicity to Terrestrial Organisms

No data were located.

Determination of PNECs

PNEC_{aquatic}: Experimental results are available for one trophic level. An acute LC₅₀ value is available for the invertebrate *Daphnia* (42 mg/L). On the basis that the data consists of only one short-term result from one trophic level, an assessment factor of 1,000 has been applied to the reported effect concentration of 42 mg/L for *Daphnia*. The PNEC_{aquatic} is 0.042 mg/L.

PNEC_{sediment}: No experimental toxicity data on sediment organisms are available. The Kow and Koc of guar gum cannot be calculated using EPISUITE because the molecular weight of guar gum greatly exceeds the limit of 1,000. Thus, the equilibrium partition

method cannot be used to determine a PNEC_{sediment} 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 Kow and Koc of guar gum cannot be calculated using EPISUITE because the molecular weight of guar gum greatly exceeds the limit of 1,000. Thus, the equilibrium partition method cannot be used to determine a PNEC_{soil} and the assessment of this compartment will be covered by the aquatic assessment.

PBT Assessment

No biodegradation was found on guar gum. However, guar gum is a naturally occurring polysaccharide which would be expected to readily biodegrade. 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 it is also water soluble. Thus, guar gum is not expected to meet the criteria for bioaccumulation.

The acute aquatic toxicity of guar gum is >0.1 mg/L. Thus, guar gum is not expected to meet the screening criteria for toxicity.

The overall conclusion is that guar gum is not a PBT substance.

References

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Environmental Assessment

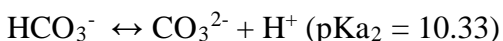
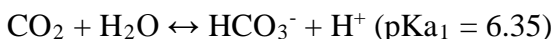
Hydrochloric acid (CAS No. 7647-01-0)

Hydrochloric acid has been reviewed in the OECD-SIDS program (OECD, 202a,b).

Environmental Fate and Transport

Hydrochloric acid is readily dissociated in water into hydrated protons and chloride ions.

The increase in the concentration of hydrochloric acid in water decreases the pH in the aquatic ecosystem. Generally, the buffer capacity to maintain the pH in the aquatic ecosystem is important and the equilibrium between CO_2 , HCO_3^- and CO_3^{2-} in the aquatic ecosystem is mainly responsible for the buffer capacity of receiving water.



According to UNEP (1995), the mean, the 10th-percentile and the 90th-percentile of bicarbonate concentrations for 77 rivers in North-America, South-America, Asia, Africa, Europe and Oceania were 106, 20 and 195 mg/L, respectively. The buffering capacity for neutralization of receiving water with bicarbonate concentrations of 20, 106 and 195 mg/L is calculated to be 2.19, 11.60 and 21.3 mg/L, respectively.

Aquatic Toxicity

Several studies on the acute toxicity to fish have been published. The lowest 96-hour LC_{50} was reported to be 4.92 mg/L for *Cyprinus carpio* at pH 4.3 which was conducted according to OECD 203 guidelines (MLIT, 1999). The 96-hour LC_{50} for *Oncorhynchus mykiss* was 7.45 mg/L at pH 4.12 for hard water and 10.3 mg/L at pH 3.98 for soft water (Graham and Wood, 1981). The 96-hour LC_{50} in *Lepomis macrochirus* is 55.1 to 30.9 mg/L at pH 3.25 - 3.5; the low pH caused a reduction in the oxygen carrying capacity of hemoglobin and excessive secretion of mucus from the gills which in turn interfered with gas exchange (Ellgaard and Glimore, 1984).

Generally, the results of toxicity tests with acid or base depend on the buffer capacity of the test medium. Dechlorinated tap water was used as a test medium in the three tests described above. A 96-hour LC_{50} of 30.9 to 24.6 at pH 3.5-3.6 was obtained for *Lepomis macrochirus* using artificial water prepared from distilled water and analytical or reagent grade chemicals (Cairns and Scheier, 1959); other reported values are a 96-hour LC_{50} of 282 mg/L for *Gambusia affinis* (Wallen *et al.*, 1957) and a 16-hour LC_{100} value of 0.492 mg/L at pH 5.3 for the pike perch fry (*Lucioperca lucioperca*) conducted with pond water

(pH 6.0-8.2) are reported (Stangenberg, 1975). A 24-hr LC₅₀ value of 60-80 mg/L for *Semotilus atromaculatus* with river water (pH 8.3) has also been reported. No long-term or chronic toxicity data on fish were located (Gillette *et al.*, 1952).

The 48-hour EC₅₀ for *Daphnia magna* is 0.492 mg/L at pH 5.3 based on immobilization (MLIT, 1999). No long-term or chronic toxicity data on invertebrates have been reported. The 72-hour EC₅₀ to *Selenastrum capriornutum* is 0.78 mg/L (pH 5.1) for biomass; 0.492 mg/L (pH 5.3) for growth rate; and the 72-hr-NOEC is 0.097 mg/L (pH 6.0) for biomass and growth rate (MLIT, 1999).

The hazard of hydrochloric acid for the environment is caused by the proton (pH effect). For this reason the effect of hydrochloric acid on the organisms depends on the buffer capacity of the aquatic ecosystem. Also, the variation in acute toxicity for aquatic organisms can be explained to a significant extent by the variation in buffer capacity of the test medium. For example, LC₅₀ values of acute fish toxicity tests varied from 4.92 to 282 mg/L.

It is not considered useful to calculate a PNEC 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.

Toxicity to Terrestrial Organisms

No data are available.

Determination of PNECS

PNEC_{aquatic}: Based on the information above, a PNEC_{aquatic} was not derived for hydrochloric acid.

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 hydrochloric acid. Thus, the equilibrium partitioning method cannot be used to calculate the PNEC_{sediment}. Based on its properties, no adsorption of hydrochloric acid 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 terrestrial organisms are available. Sorption of hydrochloric acid 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 hydrochloric acid. Thus, the equilibrium partitioning method cannot be used to calculate the PNEC_{soil}. Based on its properties, hydrochloric acid is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

PBT Assessment

Hydrochloric acid is an organic 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 most water, soil and sediment. Thus, the persistent criteria is 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; however, the acute EC(L)_{50s} are >0.1 mg/L in fish, invertebrates and algae. Thus, hydrochloric acid does not meet the screening criteria for toxicity.

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

References

Cairns, J., and Scheier, A. (1959). The relationship of bluegill sunfish body size to tolerance for some common chemicals. Proc. 13th Ind. Waste Conf., Purdue Univ. Eng. Bull. 96: 243-252.

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Environmental Assessment

Magnesium chloride (CAS No. 7786-30-3)

Environmental Fate

Magnesium chloride dissociates completely in water to the Mg^{++} cation and the chloride anion (Cl^-).

Aquatic Toxicity

The 96-hour LC_{50} of magnesium chloride to *Pimephales promelas* is 541 mg of Mg/L (or 2,119.3 mg of $MgCl_2/L$).

The 48-hour LC_{50} for *Daphnia magna* is 140 mg Mg/L (or 548.4 mg of $MgCl_2/L$). In another study, the 48-hour LC_{50} to *Daphnia magna* and *Ceriodaphnia dubia* were 339 mg of Mg/L and 225 mg of Mg/L , respectively (or 1328 and 881.4 mg of $MgCl_2/L$, respectively).

The 72-hour EC_{50} of magnesium chloride for algae *Scenedesmus subspicatus* is >100 mg/L and the $NOEC$ is 100 mg/L .

Determination of PNECs

$PNEC_{aquatic}$: Experimental results are available for three trophic levels. Acute $E(L)C_{50}$ values are available for fish (2,119 mg/L as $MgCl_2$), *Daphnia* (548 mg/L as $MgCl_2$), and algae (100 mg/L $MgCl_2$). Even though a $NOEC$ was obtained from the algae study, there were no chronic studies conducted on fish or *Daphnia*. 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 effect concentration of 100 mg/L for algae. The $PNEC_{aquatic}$ was calculated to be 0.1 mg/L . The $PNEC_{aquatic}$ is 0.1 mg/L .

$PNEC_{sediment}$: No experimental toxicity data on sediment organisms are available. Magnesium chloride dissociates completely in water with its environmental distribution is dominated by its high water solubility. Kow and Koc parameters do not readily apply to inorganics, such as magnesium chloride. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{sediment}$. Based on its properties, no adsorption of magnesium chloride 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 terrestrial organisms are available. The environmental distribution of magnesium chloride is dominated by its water solubility.

Sorption of magnesium chloride 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 magnesium chloride. Thus, the equilibrium partitioning methods cannot be used to calculate the $PNEC_{soil}$. Based on its properties, magnesium chloride is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

PBT Assessment

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; both magnesium and chloride ions are also ubiquitous and are present in most water, soil and sediment. Thus, the persistent criteria is not considered applicable to this inorganic salt.

Magnesium and chloride ions are essential to all living organisms and their intracellular and extracellular concentrations are actively regulated. Thus, magnesium chloride is not expected to bioaccumulate.

No chronic toxicity data exist on magnesium chloride; however, the acute $EC(L)_{50}$ s are >0.1 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.

Reference

ECHA REACH database: <http://apps.echa.europa.eu/registered/registered-sub.aspx>

Environmental Assessment

Polyethylene Glycol (CAS No. 25322-68-3)

Polyethylene glycols (PEGs) 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. PEGs are available in average molecular weights ranging from 200 to 8000.

No information on the aquatic toxicity and environmental fate and transport could be located for the PEGs. There are, however, data available on tetraEG and pentaEG, both being major constituents of the low molecular weight PEG 200. PEG 200 is a mixture consisting of ethylene glycols with an average molecular weight of approximately 200; there is an average of 4 oxyethylene units, but the range is from 2 to 8 oxyethylene units. The approximate composition of PEG 200 is as follows: 3% diethylene glycol (DEG), 17% triethylene glycol (TEG), 29% tetraEG, 25% pentaEG, 16% hexaEG, 8% heptaEG, and 2% octaEG (Bailey and Koleske, 1966).

Environmental Fate and Transport

PEG is a water-soluble polymer with molecular weights ranging from 200 to 8,000. PEG 200 consists of approximately 29% tetraEG and 25% pentaEG. A Mackay III fugacity model predicts that tetraEG and pentaEG will essentially distribute to water (45.3%) to soil (54.6%) (OECD, 2004).

Biodegradation

Both tetraEG and pentaEG are inherently biodegradable. For tetraEG, there was 22% degradation after 20 days in a BOD test and 40% degradation after 28 days in an OECD 301D test (Waggy *et al.*, 1994). For pentaEG, there was 34% degradation after 20 days in a BOD test (OECD, 2004).

Bioaccumulation

The log K_{ow} values for the PEG polymers were not found. Log K_{ow} and BCF values were estimated for tetraEG and pentaEG, the major constituents of the low molecular weight PEG 200. The log K_{ow} values for tetraEG and pentaEG were estimated to be -2.0 and -2.3, respectively, using EPISUITE v.4.11. The BCF values were estimated to be 3.16 for both tetraEG and pentaEG.

Aquatic Toxicity

No aquatic toxicity data were found on the PEG polymers. However, data are available on tetraEG and pentaEG.

For tetraEG, the acute 96-hour LC₅₀ to fathead minnows (*Pimephales promelas*) is >10,000 mg/L (OECD, 2004), and the acute 48-hour LC₅₀ to *Daphnia magna* is 7,746 mg/L (OECD, 2004).

For pentaEG, the acute 96-hour LC₅₀ to fathead minnows (*Pimephales promelas*) is >50,000 mg/L (OECD, 2004); the acute 48-hour LC₅₀ to *Daphnia magna* is >20,000 mg/L (OECD, 2004); and the 72-hour EC₅₀ to algae *Pseudokirchneriella subcapitata* is >100 mg/L; the NOEC is 100 mg/L (OECD, 2004).

A 7-day LC₅₀ for triethylene glycol in guppies was reported to be 63,000 mg/L (Könemann, 1981).

Toxicity to Terrestrial Organisms

No data were located on either PEG 200 or on the higher ethylene glycols, such as tetraEG and pentaEG.

Determination of PNECs

PNEC_{aquatic}: Experimental results are available for three trophic levels for PEG 200 constituents tetraEG and pentaEG. Acute E(L)C₅₀ values are available for fish (>10,000 mg/L), *Daphnia* (7,746 mg/L), and algae (>100 mg/L). Chronic toxicity data on pentaEG are available for algae (NOEC = 100 mg/L); and a chronic fish toxicity study has been conducted on triethylene glycol (NOEC = 63,000 mg/L), which is also found in PEG 200 but at lower concentrations than either tetraEG or pentaEG. 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 short-term EC₅₀ of 100 mg/L for algae. The PNEC_{aquatic} was calculated to be 2.0 mg/L.

PBT Assessment

No biodegradation data could be found on the PEG polymers. PEG is a water-soluble polymer, with molecular weights ranging from 200 to 8,000. The high molecular weight PEGs would be expected to meet the screening criteria for persistence. TetraEG and pentaEG are major constituents of the low molecular weight PEG 200. Biowin 2 predicts that both tetraEG and pentaEG will not biodegrade fast and Biowin 3 predicts the ultimate biodegradation timeframe is in weeks. Thus, the low molecular weight PEGs do not meet the screening criteria for persistence.

No information on log K_{ow} or BCF could be found on the PEG polymers. The molecular weights of PEGs range from 200 to 8,000. The high molecular weight PEGs would not be expected to bioaccumulate due to limitations in bioavailability because of the size of the polymer. TetraEG and pentaEG are major constituents of the low molecular weight PEG 200. The log K_{ow} values for tetraEG and penta were estimated to be -2.0 and -2.3, respectively; the BCF values were estimated to be 3.16 for both tetraEG and pentaEG. Thus, the low molecular weight PEGs are also not expected to meet the criteria for bioaccumulation.

No aquatic toxicity data could be located for the PEG polymers. The molecular weights of PEGs range from 200 to 8,000. The high molecular PEGs are not expected to meet the screening criteria of toxicity because the molecular size would limit bioavailability. TetraEG and pentaEG are major constituents of the low molecular weight PEG 200. There are no chronic aquatic toxicity on tetraEG or pentaEG; however, the acute aquatic toxicity is >0.1 mg/L. Thus, the low molecular weight PEGs are also not expected to meet the screening criteria for toxicity.

The overall conclusion is that the polyethylene glycol polymers are not PBT substances.

References

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Waggy, G.T., Conway, R.A., Hansen, J.L., and Blessing, R.L. (1994). Comparison of 20-d BOD and OECD closed-bottle biodegradation tests. *Environ. Toxicol. Chem.* 13: 1277-1280.

Environmental Assessment

**Benzenesulfonic acid, 4-ethytenyl-, sodium salt, homopolymer
(CAS No. 25704-18-1)**

**Acetic acid ethenyl ester, polymer with ethanol
(CAS No. 25213-24-5)**

**Vinylidene chloride/methacrylate copolymer
(CAS No. 25038-72-6)**

**Polyvinyl acetate, partially hydrolyzed
(CAS No. 30443-60-5) THIS IS NOT THE CORRECT CASRN**

All of these substances are polymers. Aquatic toxicity data was located for only for acetic acid, ethenyl ester, polymer with ethanol (CAS No. 25213-24-5) on a supplier's MSDS. However, all of the polymers listed above are expected to exhibit similar environmental fate and aquatic toxicity (Boethling and Nabholz, 1997).

Biodegradation

Generally, polymers are considered to be essentially non-biodegradable.

Bioaccumulation

Polymers are not generally absorbed through biological membranes to bioaccumulate in tissues.

Aquatic Toxicity

These polymers are not very insoluble in water and are expected to be essentially non-toxic to aquatic organisms.

The MSDS for DuPont's product ELVANOL 60-30, a polyvinyl alcohol with CAS No. 25213-24-5 (>93%) reported that concentrations of "ELVANOL" up to 10,000 mg of liter of water showed no mortality or other effect when tested on bluegill sunfish.

Determination of PNECs

PNEC_{aquatic}: Not determined.

PBT Assessment

These polymers are not expected to biodegrade and thus meets the criteria for persistence.

Polymers are not generally absorbed through biological membranes to bioaccumulate in tissues. Thus, these polymers do not meet the criteria for bioaccumulation.

The acute aquatic toxicity to fish (LC₅₀ of >10,000 mg/L) for CASRN 25213-24-5 indicates that these polymers do not meet the criteria for toxicity.

Thus, these polymers are not considered to be PBT substances.

References

Boethling, R.S. and Nabholz, J.V. (1997). Environmental Assessment of Polymers under the U.S. Toxic Substances Control Act. In: Ecological Assessment of Polymers Strategies for Product Stewardship and Regulatory Programs (Hamilton, J.D. and Sutcliffe, R. eds.), pp. 187-234, Van Nostrand Reinhold.

DuPont (2006) MSDS for “ELVANOL” 60-30, revised 27-Oct-2006.

Environmental Assessment

Sodium hydroxide (CAS No. 1310-73-2)

Sodium hydroxide (NaOH) has been reviewed in the OECD-SIDS program (OECD, 2002a,b).

Environmental Fate

The high water solubility and low vapor pressure indicate that sodium hydroxide (NaOH) will be found predominantly in the aquatic environment. NaOH is present in the environment as sodium (Na^+) and hydroxyl (OH^-) ions, which implies that it will not adsorb on particulate matter or surfaces and will not accumulate in living tissues.

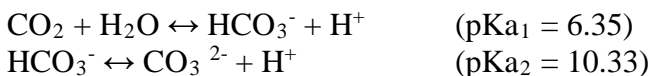
Measured concentrations in aquatic ecosystems

The concentration of hydroxyl ions in the environment has been determined very extensively via pH measurements. The pH is a very important parameter of aquatic ecosystems and it is a standard parameter of water quality monitoring programs. The most important freshwater aquatic ecosystems of the world revealed average annual pH values between 6.5 and 8.3 but lower and higher values have been measured in other aquatic ecosystems (UNEP, 1995). In aquatic ecosystems with dissolved organic acids a pH of less than 4.0 has been measured, while in waters with a high chlorophyll content the bicarbonate assimilation can result in pH values of higher than 9.0 at midday (UNEP, 1995). The pH of an aquatic ecosystem is mainly determined by geochemical, hydrological and/or biological processes.

Also sodium has been measured extensively in aquatic ecosystems. For example UNEP (1995) reported the concentration for a total number of 75 rivers in North-America, South-America, Asia, Africa, Europe and Oceania. The 10th –percentile, mean and 90th-percentile were 1.5, 28 and 68 mg/l, respectively.

NaOH addition and buffer capacity

An addition of NaOH 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-} :



If the pH is between 7 and 9 then the bicarbonate ion is the most important species responsible for the buffer capacity of aquatic ecosystems. UNEP (1995) reported the bicarbonate concentration for a total number of 77 rivers in North-America, South-America, Asia, Africa, Europe and Oceania. The 10th– percentile, mean and 90th-percentile were 20, 106 and 195 mg/l, respectively.

Aquatic Toxicity

At concentrations reported in publications and study reports, the toxicity has been assumed to be due to hydroxide only, because at these effect concentrations the concentration of sodium is too low to explain the effects. However, it should be realized that the results of toxicity tests with NaOH depend on the buffer capacity of the test medium. In a highly buffered test medium the hydroxyl ion will be neutralized and the observed toxicity will be low, while in a poorly buffered test medium the pH will increase rapidly and therefore the observed toxicity will be relatively high. Besides the direct effects (pH change) NaOH could also have indirect effects. The pH change could influence the speciation of other chemicals and therefore increase and/or decrease the toxicity *e.g.*, NH₃ is more toxic than NH₄⁺.

The 24-hour LC₅₀ 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 LC₅₀ to *Leuciscus idus melanotus*, is 189 mg/L. The 96-hour LC₅₀ 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. The 48-hour LC₅₀ 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.

No data are available on the effects of NaOH on algae.

Toxicity to Terrestrial Organisms

Toxicity tests, which determined the effects of NaOH on terrestrial organisms, are not available. Significant exposure of the terrestrial environment is not expected and for this reason there is no need to perform toxicity test with terrestrial organisms. The results of terrestrial toxicity tests will depend strongly on the buffer capacity of the soil and can probably be predicted based on the buffer capacity of the soil.

Determination of PNECs

In many cases pH, buffer capacity and/or medium composition were not discussed in the publications, although this is essential information for toxicity tests with NaOH. This is the most important reason why most of the studies, mentioned above were considered invalid. Although valid acute ecotoxicity tests and chronic ecotoxicity tests with NaOH are not available there is no need for additional testing with NaOH. A significant number of acute toxicity tests are available and the results of the tests are more or less consistent. Altogether they give a sufficient indication about acute toxicity levels of sodium hydroxide.

Furthermore acute toxicity data cannot be used to derive a PNEC or a PNEC added for sodium hydroxide. Aquatic ecosystems are characterized by an alkalinity/pH and the organisms of the ecosystem are adapted to these specific natural conditions. Based on the natural alkalinity of waters, organisms will have different optimum pH conditions, ranging from poorly buffered waters with a pH of 6 or less to very hard waters with pH values up to 9. A lot of information is available about the relationship between pH and ecosystem structure and also natural variations in pH of aquatic ecosystems have been quantified and reported extensively in ecological publications and handbooks.

Normally a PNEC or a PNEC added has to be derived from the available ecotoxicity data. A PNEC added is a PNEC which is based on added concentrations of a chemical (added risk approach). Based on the available data it is not considered useful to derive a PNEC or a PNEC added for NaOH because:

- The natural pH of aquatic ecosystems can vary significantly between aquatic ecosystems,
- Also the sensitivity of the aquatic ecosystems to a change of the pH can vary significantly between aquatic ecosystems and
- The change in pH due to an anthropogenic NaOH addition is influenced significantly by the buffer capacity of the receiving water.

Although a PNEC or a PNEC added was not calculated for NaOH there is a need to assess the environmental effect of an NaOH (alkaline) discharge. Based on the pH and buffer capacity of effluent and receiving water and the dilution factor of the effluent, the pH of the receiving water after the discharge can be calculated. Of course the pH change can be measured also very easily via a laboratory experiment or by conducting field measurements. The change in pH should be compared with the natural variation in pH of the receiving water and based on this comparison it should be assessed if the pH change is acceptable.

$PNEC_{\text{aquatic}}$: Based on the information above, a PNEC was not derived for sodium hydroxide.

$PNEC_{\text{sediment}}$: No experimental toxicity data on sediment organisms are available. Sodium hydroxide 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 sodium hydroxide. Thus, the equilibrium partitioning method cannot be used to calculate the $PNEC_{\text{sediment}}$. Based on the its properties, no adsorption of sodium hydroxide to sediment is to be expected, and the assessment of this compartment will be covered by the aquatic assessment.

$PNEC_{\text{soil}}$: No experimental toxicity data on terrestrial organisms are available. The environmental distribution of sodium hydroxide is dominated by its water solubility.

Sorption of sodium hydroxide 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 hydroxide. Thus, the equilibrium partitioning method cannot be used to calculate the PNEC_{soil}. Based on its properties, sodium hydroxide is not expected to significantly adsorb to soil, and the assessment of this compartment will be covered by the aquatic assessment.

PBT Assessment

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 is 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.

No chronic toxicity data exist on sodium hydroxide; however, the acute EC(L)_{50s} are >0.1 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.

References

OECD (2002a). IUCLID Data Set for Sodium hydroxide (CAS No. 1310-73-2), UNEP Publications.

OECD (2002b). Screening Information Dataset (SIDS) Initial Assessment Report for Sodium hydroxide (CAS No. 1310-73-2), UNEP Publications.

Environmental Assessment

Talc (CAS No. 61789-40-0)

Talc is a mineral composed of hydrated magnesium silicate with the chemical formula $\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$ or $\text{H}_2\text{Mg}_3(\text{SiO}_3)_4$. Talc is not soluble in water.

Biodegradation

As a mineral, talc does not biodegrade.

Aquatic Toxicity

No data were found. As an insoluble mineral, talc is not expected to be bioavailable; therefore, it is not expected to be toxic to aquatic organisms.

Toxicity to Sediment Organisms

No data were found. As an insoluble mineral, talc is not expected to be bioavailable; therefore, it is not expected to be toxic to sediment organisms.

Toxicity to Terrestrial Organisms

No data were found.

Determination of PNECs

PNEC values for talc cannot be calculated.

PBT Assessment

Talc is an inorganic mineral that is insoluble in water. Talc is not expected to be bioavailable to aquatic organisms; thus, it does not meet the criteria for bioaccumulation or toxicity. Talc does not biodegrade in the environment. It is a naturally-occurring mineral and is persistent in the environment. However, for the purposes of this PBT assessment, it does not meet the criteria for persistence.

Environmental Assessment

Tetrasodium ethylenediaminetetraacetate (CAS No. 64-02-8)

An EU Risk Assessment Report was completed for tetrasodium ethylenediaminetetraacetate (2004).

Environmental Transport

As no value for the vapor pressure is known, a Henry's law constant cannot be calculated from vapor pressure and water solubility. Because of the ionic properties of ethylenediaminetetraacetate (EDTA) and its metal complexes, it has to be assumed that volatilization from aqueous solution will not occur. Due to the ionic structure under environmental relevant pH conditions, no adsorption onto the organic fraction of soils or sediments is expected. In a laboratory test, the mobility of EDTA in soil was tested. A solution of H₄EDTA was eluted through cores of two various surface soils. H₄EDTA was found to be very slightly adsorbed and moved quite readily through both soils.

Based on the physico-chemical properties of H₄EDTA, a calculation with the fugacity model Mackay level I predicts that the hydrosphere is the preferred environmental compartment (99.999%).

Biodegradation

“EDTA is not readily biodegradable. The results of different tests on inherent biodegradability are unequal. The available, not well documented tests show for instance biodegradation rates from 0 and 37% under application of pre-adapted inoculum after 14 days. In a Modified Zahn-Wellens Test (OECD 302 B) a biodegradation of < 20% could be found after 28 days with non-adapted sludge.”

“Recent data suggest that under alkaline conditions EDTA can be degraded. Environmental samples from a river, a ditch and a lake were examined in the Closed Bottle test for their potential to degrade CaNa₂EDTA in a concentration of 8.0 mg/l at pH 6.5 and 8.0 over a period of few weeks. The results show for all environmental samples that at pH 6.5 no or little biodegradation (2-12%) occurs within the first 28 days. After 49 days a biodegradation between 60 and 83% was obtained. At pH 8, rates of 53, 62 and 72% were obtained after 28 days and 75-89% after 35 days.”

“Results obtained at pH of 8 could be relevant because the pH value of lake and river water ranges from 7.7 to 8.5. However, in surface waters, EDTA is preferably complexed with heavy metal ions. Regarding the degradation tests cited above, no biological degradation is expected. Ca-EDTA can only occur in the environment where strong point

sources release this species into a river with a low flow. Therefore, in the present exposure assessment EDTA is regarded as not biodegradable in surface waters, and a biodegradation rate constant of 0 d⁻¹ is used.”

Bioaccumulation

“Bishop and Maki (1980) studied bioaccumulation of EDTA on the fish *Lepomis macrochirus*, using the kinetic and the plateau method. Under actual requirements only the results of the plateau method can be used. After 28 days, the EDTA level in the fish, as determined by the plateau method, was of the same order of magnitude as the level in the ambient water. Depending on the used concentration BCF of 1.8±1.1 (0.08mg/l EDTA) and 1.1±0.95 (0.76 mg/l EDTA) could be obtained. From this data it can be concluded that no bioaccumulation takes place.”

Aquatic Toxicity

“Most of the acute tests performed with fish and daphnids revealed LC/EC₅₀ values well above 100 mg/L, indicating for complexed and non complexed EDTA no need for classification as dangerous for the environment. Exceptions are two fish tests using H₄EDTA, where the tests were performed in very soft (LC₅₀ = 41 mg/L) or soft water (LC₅₀ = 59.8 mg/L). In the test media a surplus of uncomplexed EDTA was present which is not expected in the environment, therefore this tests are not relevant for the assessment.”

“Tests on acute toxicity with *Daphnia magna* resulted in 24-hr EC₅₀ values of 480 and 790 mg/L.”

“Algae tests performed in standard media resulted in effect values below 1 mg/L. The effect is probably caused by nutrient deficiency. This indirect effect is an artifact and not used in the effects assessment. Further experiments with increased nutrient metal concentrations reveal that the direct toxicity on algae is above 310 mg/L. Indirect effects like nutrient deficiency and eutrophication could only qualitatively be assessed; they are unlikely to occur in the environment although it cannot absolutely be excluded.”

Determination of PNEC_{aquatic}

“According to the results from different ecotoxicological studies discussed above, the toxicological profile of EDTA is based on disturbances of metal metabolism. For the interpretation of toxicity tests, the complex formation properties of EDTA have to be taken into account.”

“Beside Ca and Mg, test media contain a certain amount of heavy metal ions being necessary as trace nutrients. The complex forming constants of heavy metal complexes

are by several orders of magnitude higher than of Ca/Mg-complexes, thus after addition of the test substance EDTA (as acid or Na-salt) the concentration of uncomplexed trace metals decreases drastically. The degree of Ca/Mg complexation is dependent on the amount of added EDTA. Uncomplexed EDTA is only present when it is present in overstoichiometric concentrations.”

“The choice of the complex species being relevant for effect testing should consider their different ecotoxicological properties. A mixture of metal complexes is always released or is being formed in surface waters. Effect tests should be conducted with a complex for which metal toxicity can be excluded. We propose to use the Ca-complex as test substance for all release scenarios. Effects from complexes with a higher toxicity are caused by the dissociated metal ions and should be covered by the risk assessment of the respective metals.”

“Short-term tests on fish reveal that EDTA and Na-EDTA are more toxic in an uncomplexed form. This can only occur if they are available in over-stoichiometric amounts to the chelants. Under these conditions the complexing agents can cause nutrient deficiency by reducing the essential concentration of different ions. The higher the water hardness the higher was the concentration of EDTA necessary to cause a toxic effect expressed as mortality: 96-hr LC₅₀ values for H₄EDTA between 41 mg/L and 1590 mg/L were found. The lowest acute toxicity recorded with H₄EDTA for the fish *Lepomis macrochirus* in very soft water with LC₅₀ of 41 mg/L should not be used because it is probably influenced by pH effects. In the test result obtained with Na-EDTA and a water hardness of 103 mg/L CaCO₃ (96-hr LC₅₀ = 374 mg/L) pH effects of the acid are completely suspended. However, uncomplexed EDTA was applied in a stoichiometric excess which is in contrast to environmental conditions. Using CaNa₂EDTA as test substance, a LC₅₀ of 1,827 mg/L was obtained being in a concentration range where unspecific effects are expected. The results of the test with *Pimephales promelas* (96-hour LC₅₀ = 59.8 mg/L, obtained in water hardness of 40-48 mg/l CaCO₃ are doubtful, as the effects might have been caused by a low pH value. All tests on acute fish toxicity are of limited relevance for the PNEC derivation.”

“In an early-life stage test on the zebrafish *Danio rerio*, the NOEC was determined to > 26.8 mg/L H₄EDTA based on analytically determined concentrations. CaNa₂EDTA was used as test substance. This test is considered to be the most relevant fish test for the PNEC derivation.”

“For daphnids no investigation on the influence of water hardness or possible reduced nutrient conditions are available. The available acute tests are carried out by in hard water (160 mg/l CaO). It is known, that calcium deficiency inhibited the development of fresh water crawfish. 24-hr EC₅₀ values of 480 to 790 mg/L for *Daphnia magna* were found. In a long-term test a 21-day NOEC of 22 mg/l for reproduction could be obtained. In the latter test a surplus of Ca was present, thus mainly Ca-EDTA was formed in the medium being the active test substance.”

“The apparent effects of complexing agents to algal growth are related to essential trace metal bioavailability. Trace metal levels tend to be more important in algae tests than in short-term tests on fish or daphnia, the main reason is the rapid increase of biomass during the test. It was demonstrated that not the absolute EDTA concentration, but rather the ratio of the EDTA concentration to the metal cations is crucial to algae growth. With sufficient trace metal amounts, H₄EDTA concentrations up to 310 mg/L caused no effects. Similar results are obtained when Fe(III)EDTA is used as test substance, due to its slow metal exchange kinetics overchelation of the nutrient metal ions is avoided. Therefore direct effects caused by the intrinsic toxicity of EDTA are not expected in surface waters, where in nearly every case a stoichiometric surplus of metal ions is present.”

“A standard growth inhibition test on *Scenedesmus subspicatus* resulted in an EC₁₀ of 0.37 mg/L H₄EDTA. The effect is probably caused by nutrient deficiency, as essential metal ions like Cu, Zn and Co are largely complexed leading to drastically reduced concentrations. In a test with *Pseudokirchnerella subcapitata* (formerly *Selenastrum capricornutum*) with Fe(III)EDTA as an active test substance following OECD TG 201, EC₅₀ and EC_{r50} higher than 100 mg/L were found. The NOEC based on nominal concentrations was determined to 79.4 mg/L and to 48.4 mg/L when based on mean measured concentration.”

“Therefore, this inhibition of algae growth is an artifact which is caused by the drastic increase of biomass during the test. Indirect effects cannot be quantified from the laboratory tests, thus only theoretical considerations can be made. In German and Dutch rivers, heavy metal concentrations in the range of 10-20 µmol/L (predominantly Fe and Mn) are detected. In the environment heavy metals are generally present in over-stoichiometric amounts, thus those effects are not expected in low concentrations like in the tests. Nutrient deficiency in surface waters can only occur when essential metal ions are overchelated by high EDTA amounts. On the other hand, plant growth is influenced by many limiting parameters; probably the presence of macronutrients like phosphate or nitrate is of greater importance. Therefore, it is unlikely that nutrient deficiency occurs in the environment, although it cannot be excluded absolutely.”

“In addition to the discussed adverse effects, like growth inhibition, mortality and immobilization of EDTA the growth stimulating effects like eutrophication occurs. Standard media for algae tests contain EDTA (OECD 201: 100 µg/L) to prevent precipitation of nutrient metals as hydroxide. For two different river waters a significant increase in phytoplankton production was observed after addition of 30 to 300 µg/L EDTA. The observed increase in growth varied with algae species, preloading of the water with trace elements and other complexing agents e.g. humic acids from 22 to 50%. Thus, the higher availability of trace elements through the complexing agent EDTA depends on the preloading of the water and can significantly stimulate the processes of eutrophication. If trace elements like Fe, Co, Mn, and Zn are sufficiently available in a soluble form, the algae growth will be increased after addition of EDTA only insignificantly. This aspect of effects cannot be assessed quantitatively with the available methods.”

“The effects assessment of EDTA is based on long-term tests, which are available for fish, daphnids and algae. The most sensitive endpoint could be found for *Daphnia magna* with a NOEC of 22 mg/L H₄EDTA. According to TGD an assessment factor of 10 has to be used.”

The PNEC_{aquatic} is 2.2 mg/L.

Determination of PNEC_{sediment}

“There are no test results available with sediment dwelling organisms. A determination of the PNEC sediment is not possible. Based on the properties no adsorption of EDTA onto the sediment has to be expected, thus the assessment of this compartment will be covered by the aquatic assessment.”

Determination of PNEC_{soil}

“There are only test results available which investigate the decrease of heavy metal toxicity caused by EDTA. It is not possible to derive a PNEC with this data. Therefore, the assessment can be based on the pore water concentration only.”

Reference

EU (2004). European Union Risk Assessment Report for Tetrasodium ethylenediamineacetate (CAS No. 64-02-8), Volume 51.