National assessment of chemicals associated with coal seam gas extraction in Australia

Technical report number 14

Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia: Appendices A, B, C, D, F, and G

This report was prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy

Australian Government
Department of the Environment and Energy
Department of Health
National Industrial Chemicals Notification and Assessment Scheme

The national assessment of chemicals associated with coal seam gas extraction in Australia was commissioned by the Department of the Environment and Energy and prepared in collaboration with NICNAS and CSIRO

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2	Literature review: Human health implications	NICNAS
3	Literature review: Environmental risks posed by chemicals used coal seam gas operations	Department of the Environment and Energy
4	Literature review: Hydraulic fracture growth and well integrity	CSIRO
5	Literature review: Geogenic contaminants associated with coal seam gas operations	CSIRO
6	Literature review: Identification of potential pathways to shallow groundwater of fluids associated with hydraulic fracturing	CSIRO
	Identifying chemicals used in coal seam gas extraction	
7	Identification of chemicals associated with coal seam gas extraction in Australia	NICNAS
	Modelling how people and the environment could come into contact with chemicals during coal seam gas extraction	
8	Human and environmental exposure conceptualisation: Soil to shallow groundwater pathways	CSIRO
9	Environmental exposure conceptualisation: Surface to surface water pathways	Department of the Environment and Energy
10	Human and environmental exposure assessment: Soil to shallow groundwater pathways – A study of predicted environmental concentrations	CSIRO

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	Assessing risks to workers and the public	
11	Chemicals of low concern for human health based on an initial assessment of hazards	NICNAS
12	Human health hazards of chemicals associated with coal seam gas extraction in Australia	NICNAS
13	Human health risks associated with surface handling of chemicals used in coal seam gas extraction in Australia	NICNAS
	Assessing risks to the environment	
14	Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia	Department of the Environment and Energy

Foreword

Purpose of the Assessment

This report is one in a series of technical reports that make up the *National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia* (the Assessment).

Many chemicals used in the extraction of coal seam gas are also used in other industries. The Assessment was commissioned by the Australian Government in June 2012 in recognition of increased scientific and community interest in understanding the risks of chemical use in this industry. The Assessment aimed to develop an improved understanding of the occupational, public health and environmental risks associated with chemicals used in drilling and hydraulic fracturing for coal seam gas in an Australian context.

This research assessed and characterised the risks to human health and the environment from surface handling of chemicals used in coal seam gas extraction during the period 2010 to 2012. This included the transport, storage and mixing of chemicals, and the storage and handling of water pumped out of coal seam gas wells (flowback or produced water) that can contain chemicals. International evidence[1] showed the risks of chemical use were likely to be greatest during surface handling because the chemicals were undiluted and in the largest volumes. The Assessment did not consider the effects of chemical mixtures that are used in coal seam gas extraction, geogenic chemicals, or potential risks to deeper groundwater.

The Assessment findings significantly strengthen the evidence base and increase the level of knowledge about chemicals used in coal seam gas extraction in Australia. This information directly informs our understanding of which chemicals can continue to be used safely, and which chemicals are likely to require extra monitoring, industry management and regulatory consideration.

Australia's regulatory framework

Australia has a strong framework of regulations and industrial practices which protects people and the environment from adverse effects of industrial chemical use. For coal seam gas extraction, there is existing legislation, regulations, standards and industry codes of practice that cover chemical use, including workplace and public health and safety, environmental protection, and the transport, handling, storage and disposal of chemicals. Coal seam gas projects must be assessed and approved under relevant Commonwealth, state and territory environmental laws, and are subject to conditions including how the companies manage chemical risk.

Approach

Technical experts from the National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the Commonwealth Scientific and Industrial Research Organisation (CSIRO), and the Department of the Environment and Energy conducted the Assessment. The Assessment drew on technical expertise in chemistry, hydrogeology, hydrology, geology, toxicology, ecotoxicology, natural resource management and risk assessment. The

[1] See Mallants et al. 2017a; Jeffrey et al. 2017; Adgate et al. 2014; Flewelling and Sharma 2014; DEHP 2014; Stringfellow et al. 2014; Groat and Grimshaw 2012; Vidic et al. 2013; Myers 2012; Rozell and Reaven 2012; The Royal Society and The Royal Academy of Engineering 2012; Rutovitz et al. 2011.

Independent Expert Scientific Committee on Coal Seam Gas and Large Coal Mining Development (IESC) provided advice on the Assessment. Experts from the United States Environmental Protection Authority, Health Canada and Australia reviewed the Assessment and found the Assessment and its methods to be robust and fit-for-purpose.

The Assessment was a very large and complex scientific undertaking. No comparable studies had been done in Australia or overseas and new models and methodologies were developed and tested in order to complete the Assessment. The Assessment was conducted in a number of iterative steps and inter-related processes, many of which needed to be done in sequence (Figure F.1). There were two separate streams of analysis – one for human health and one for the environment. The steps included for each were: literature reviews; identifying chemicals used in drilling and hydraulic fracturing for coal seam gas extraction; developing conceptual models of exposure pathways; models to predict soil, surface and shallow groundwater concentrations of identified chemicals; reviewing information on human health hazards; and identifying existing Australian work practices, to assess risks to human health and the environment.

The risk assessments did not take into account the full range of safety and handling precautions that are designed to protect people and the environment from the use of chemicals in coal seam gas extraction. This approach is standard practice for this type of assessment. In practice, safety and handling precautions are required, which means the likelihood of a risk occurring would actually be reduced for those chemicals that were identified as a potential risk to humans or the environment.

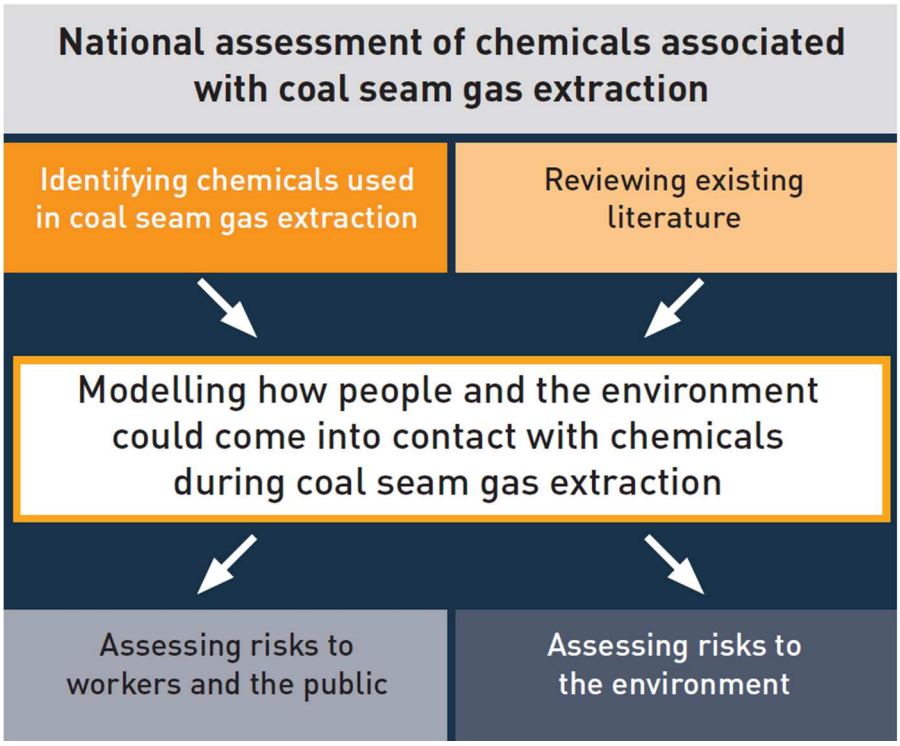

Figure F.1 Steps in the assessment

Collaborators

The Australian Government Department of the Environment and Energy designs and implements policies and programs, and administers national laws, to protect and conserve the environment and heritage, promote action on climate change, advance Australia's

interests in the Antarctic, and improve our water use efficiency and the health of Australia's river systems.

Within the Department, the Office of Water Science is leading the Australian Government's efforts to improve understanding of the water-related impacts of coal seam gas and large coal mining. This includes managing the Australian Government's program of bioregional assessments and other priority research, and providing support to the Independent Expert Scientific Committee on Coal Seam Gas and Large Coal Mining Development (IESC). The IESC provides independent, expert scientific advice on coal seam gas and large coal mining proposals as requested by the Australian Government and state government regulators, and advice to the Australian Government on bioregional assessments and research priorities and projects.

The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is a statutory scheme administered by the Australian Government Department of Health. NICNAS aids in the protection of the Australian people and the environment by assessing the risks of industrial chemicals and providing information to promote their safe use.

CSIRO, the Commonwealth Scientific and Industrial Research Organisation, is Australia's national science agency and one of the largest and most diverse research agencies in the world. The agency's research is focused on building prosperity, growth, health and sustainability for Australia and the world. CSIRO delivers solutions for agribusiness, energy and transport, environment and natural resources, health, information technology, telecommunications, manufacturing and mineral resources.

This report: *Environmental risks associated with surface handling of chemicals used in coal seam gas extraction: Appendices A, B, C, D, F, and G*

These Appendices are intended to be read in conjunction with the covering report, entitled *Environmental risks associated with surface handling of chemicals used in coal seam gas extraction* (DoEE 2017a), as they contain details of the methodology used by the Department of the Environment and Energy to complete the environmental risk assessment.

Appendix G - *Compiled qualitative risk assessments of 54 chemicals* – documents the qualitive environmental risk assessment for 54 chemicals associated with coal seam gas extraction in Australia.

A further appendix (Appendix E) is provided as a Microsoft Word workbook, detailing the results of the mathematical expressions used to quantify the potential environmental risks of chemical use (drilling and hydraulic fracturing) for coal seam gas extraction in Australia.

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Appendix A – Methodology for chemical characterisation

1 Methodology for chemical characterisation

1.1 Introduction

The chemical characterisation stage involves verifying chemical identities and collecting ecotoxicity and physico-chemical data for each chemical – information that is needed for the risk estimation models (especially for the transfer pathways and environmental receptors models) and to determine potential effects on ecosystems during the risk assessment. The general scientific literature was the main source of information for this chemical characterisation work.

The methodology used to obtain the data and the steps undertaken to establish the predicted no effect concentration (PNEC) of each chemical, which is used to calculate the Risk Quotient (RQ) and determine a chemical's potential risk, is described in this Appendix.

The list of 113 drilling and / or hydraulic fracturing chemicals was obtained from a specifically commissioned report (NICNAS 2017a), including chemical names and CAS RNs.

Data were obtained from the supplied Chemical Abstracts Services Registry Number (CAS RN) using the Organisation for Economic Cooperation and Development (OECD) Quantitative Structure Activity Relationships (QSAR) Toolbox v2.2 (OECD 2013a) and OECD QSAR Toolbox v3.1 (OECD 2013a)[2]. This included relevant measured physico-chemical properties and measured ecotoxicological data.

Where data for a specific chemical were absent, several tools were used to infer this information by interpolation or extrapolation from similar chemicals for which the information was available. To achieve this, the QSAR modelling approach (ECHA 2008) was mostly used, supplemented with the use of analogue data where appropriate.

1.2 Measured ecotoxicity data

Once all of the chemicals were uniquely and unequivocally identified, QSAR Toolbox v2.2 and v3.1 databases were interrogated to obtain ecotoxicological endpoints.

It is understood that the only difference in the databases for v2.2 and v3.1 is the inclusion of information from ECHA. However, data from ECHA (2013) has not been verified and was not used unless further verified directly by ECHA. The database contains numerous ecotoxicological endpoints for numerous species. These endpoints are a numerical summary of the study and include further details including study protocols and authors' notes. However, they still only provide limited detail of the original studies. Accordingly, the data

[2] The QSAR Toolbox software was produced by the Laboratory of Mathematical Chemistry (LMC) in cooperation with the OECD and the European Chemicals Agency (ECHA). It contains a comprehensive database of chemical identities and experimental results from the literature for thousands of chemicals.

downloaded were restricted to standard endpoints from standard tests on aquatic, sediment and terrestrial species as specified by EPHC (2009) and OECD Test Guidelines (TGs) 201, 202, 203, 210, 211. and 215, although some latitude was given in regard to test species and exact duration of the study. The endpoints generated by these studies, which are routinely used in risk assessments, are presented in Table A.1 (below).

Table A.1 Standard studies for determining endpoints

	Endpoint	**OECD TG**	**Reference**
Acute endpoints	EC50 algae (growth rate 72 or 96 h)	201	OECD (2011a)
	EC50 daphnia (immobilisation 48 h)	202	OECD (2004a)
	LC50 fish (mortality 96 h)	203	OECD (1992a)
Chronic endpoints	NOEC algae (growth rate 72 h or 96 h)	As for acute	
	NOEC daphnia (Reproduction and mortality 14–21 d)	211	OECD (2012a)
	NOEC fish (hatching, morphology, mortality up to 60 days post hatch)	210 and 215	OECD (2013b) OECD (2000b)

All values were converted to mg/L from other units using standard values for molecular weight and density (e.g. Aylward and Findlay 1974; Atkins 1986). In addition, due to the limited detail provided on the endpoints from QSAR Toolbox, a quality check was conducted on the data to determine its acceptability as described in the sub-section 'Quality' below.

1.2.1 Estimated ecotoxicity data

1.2.1.1 QSARs

Many chemicals did not have measured endpoints of interest, as studies have not been conducted (or reported). Where possible, endpoints were estimated using the QSAR modelling approach.

The QSAR modelling approach is based on the premise that molecules may be considered as fragments including single atoms and larger functional groups. These fragments may then be used to categorise the chemical into a class (e.g. esters, amines, etc.) of structurally similar compounds (Mayo-Bean et al. 2012a) and to estimate the n-octanol water partition coefficient (Kow) (Meylan and Howard 1995) of the chemical. These factors are considered to be the most influential in determining ecotoxicity (Mayo-Bean et al. 2012a, 2012b).

This analysis was conducted using ECOSAR v 1.1 (US EPA 2000-2012), which was accessed through the QSAR Toolbox. The ECOSAR model also contains the sub-program KOWWIN (US EPA 2000), which estimates the Kow of chemicals. Each chemical class (as described above) has a linear equation relating the log of the acute or chronic ecotoxicity (fish, *Daphnia*, algae and others) to the log Kow, based on a training set of chemicals in that class selected from a database of measured ecotoxicity and Kow values. Once the Kow value for a chemical is calculated, its ecotoxicity value may also be calculated from the QSAR equation for a chemical class.

As the toxicity calculation is based on the Kow of the chemical, inorganic compounds and organometallics are not amenable to this analysis, nor are some organic chemicals with

specific modes of action. Similarly, given that the analysis of QSARs is based on a physical property (Kow) unique to a discrete organic chemical, and data entry requires the identification of a discrete organic chemical, this analysis is not applicable to UVCBs (Mayo-Bean et al. 2012b).

1.2.1.2 Surfactant chemicals

Surfactant chemicals do not partition to n-octanol or water but remain at the interface between the two layers. Accordingly, a Kow, which is required for the calculation of ecotoxicity by the standard method used by ECOSAR, cannot be accurately estimated for these chemicals (Mayo-Bean et al. 2012a, 2012b). However, an estimate of ecotoxicity of surfactants based on the average chain length of the hydrophobic component and whether the surfactant is anionic (negatively charged), cationic (positively charged), non-ionic (not charged) or amphoteric (containing both a positive and a negative charge) (ibid) may be made using ECOSAR.

This approach does not, however, take into account the functional groups of the surfactant other than what charge it has, and calculates an average of the properties of UVCBs (which many surfactants are). Therefore, where ecotoxicity data from suitable analogues (see Section 1.2.1.3) were available, these were used in preference to modelled data for surfactants.

Nine chemicals were identified as surfactants and their source of the ecotoxicity data is presented in the Table A.2.

Table A.2 Surfactants and the sources of their endpoints

CAS RN	Chemical name	Analogue available *	ECOSAR special class	Estimated ECOSAR	Analogue LC50
CBI	Ethoxylated fatty acid	Yes	-	-	2.2 mg/L 96 hour on green alga
CBI	Ethoxylated fatty acid – a nonionic surfactant	Yes	-	-	5 mg/L acute daphnia
CBI	Ethoxylated fatty acid – a nonionic surfactant	No	No	Unreliable	-
CBI	Organic sulfate	Yes	-	-	0.74 acute mg/L and chronic daphnia 0.37 mg/L
68187-17-7	C_{6-10} alkyl sulfonate esters - anionic surfactant	Yes	-	-	33–39 mg/L for two acute
68439-45-2	alcohols, C_{6-12}, ethoxylated - nonionic surfactant	Yes	-	-	4.87 mg/L 96 h fish
CBI	Organic acid salt	No	Yes	-	-
81741-28-8	Phosphonium, tributyltetradecyl-,	No	Yes	-	-

CAS RN	Chemical name	Analogue available *	ECOSAR special class	Estimated ECOSAR	Analogue LC50
	chloride				

[*] *Available from Madsen et al. (2001)*

The Toolbox incorrectly assigned the structure for ethoxylated fatty acids but this was corrected. The corrected structure was regarded as the UVCB cocamide DEA, for the following reasons:

- one of the major constituents of the CBI ethoxylated fatty acids is known. The closest analogue of the major constituent and its corresponding EC50 value over an unspecified time was identified for *Daphnia*
- ecotoxicity values of an homologous series of chemicals, including organic sulfate (CBI), were identified and included a 96-hour EC50 and a 21-day NOEC for *Daphnia magna* (Madsen et al. 2001)
- ethoxylated fatty acid (CBI) is a UVCB. A suitable analogue could not be found and although ECOSAR assigned modelled values, these were considered unreliable due to variable composition and it was not modelled as a surfactant
- the surfactant C_{6-10} alkyl sulphonate esters (68187-17-7) would include C_{6-8} dialkyl sulfosuccinates. These have ecotoxicity values (EC/LC50) for daphnia and fish of 33 and 39 mg/L, respectively (ibid)
- ethoxylated C_{6-12}, alcohols (68439-45-2) increase in toxicity with their chain length. This excluded use of longer chain ethoxylated alcohols as analogues. However, a chronic study was conducted on the ecotoxicity of C_9-C_{11} ethoxylated alcohols on fathead minnow larvae for 672 h (28 days). An LC50 of 4.87 mg/L was established (ibid)
- a suitable analogue for organic acid salt (CBI) could not be found. However, the chemical class and average carbon chain length was adequately modelled by ECOSAR's special class function
- a suitable analogue for phosphonium, tributyltetradecyl chloride (81741-28-8) could not be found. However, it was classified as a phosphonium cationic surfactant with an average 6.5 carbons per chain and was adequately modelled by ECOSAR's special class function.

1.2.1.3 Use of chemical analogues

When experimental data is not available, it is appropriate to use data from analogue chemicals in certain cases. Determining whether or not this technique is applicable is based on expert judgement, and depends on the nature of the data gap that is to be filled. The basis for using analogue data is usually strong structural similarity between the chemical in question and the analogue, but other factors such as the toxicological mode of action are also taken into consideration (EPHC 2009).

If data for more than one analogue chemical is available, this data may be interpolated based on the log Kow of the analogues and the chemical under consideration. This is the basis of the QSAR modelling approach, as described above.

Analogue data may also be used to check the validity of QSAR models when data for an analogue chemical are available. Cross-checks were conducted where possible when:

- The ecotoxicity predicted by QSAR for the species in question was more than one order of magnitude greater or less than the measured ecotoxicity for other species.
- There was no measured ecotoxicity data available for the chemical in question.

Two chemicals were further checked for analogue data. The first was 1,3-propanediol, 2-bromo-2-nitro-(52517) as the QSAR data for algae and *Daphnia* was greater than one order of magnitude different from the measured value for fish. The second was 2-naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-, (6410419) for which no measured ecotoxicity data were available. The search for analogue data was conducted using QSAR Toolbox v3.1 (using the 'structure similarity' and 'category definition' functions) but no chemicals were considered closely similar enough to be regarded as analogues.

1.3 Quality

For any model, it is important to have sufficient quality input data (DoEE 2017b and 2017c). Accordingly, as part of the development of the database for chemical properties used in the environmental risk assessment, all data were assessed for quality. This involved quality assurance (the planned and systematic activities implemented in a quality system) and quality control (the examination of outputs to uncover errors and inconsistencies).

The quality assurance program was based on the Department of the Environment's internal quality assurance documentation developed for the Inventory Multi-Tiered Assessment Project (IMAP) program, which is similarly using QSAR Toolbox for the evaluation of chemical ecotoxicity [3]. Both the test and modelled data were assessed for quality, but due to the differences in origin, they were found to have different processes.

1.3.1 Quality assurance

The most critical component of quality assurance was ensuring that the data produced by QSAR Toolbox were scientifically valid and not extrapolated beyond the reported study design or its modelling capabilities. The following sub-sections outline the quality assurance procedure undertaken for test and modelled data.

1.3.1.1 Test data

As indicated previously (see Section 1.2), only data from studies from QSAR Toolbox that met OECD TG requirements were used. These guidelines also specify that knowledge of chemical properties is required such that the chemical's behaviour, including degradation, losses and solubility, in test systems is known. More specifically, EPHC (2009) and US EPA (2000-2012) specify substances that are hard to test and outline criteria to assess the quality of the data. They are:

- if it is difficult to test a substance, whether the following factors have been accounted for in the study:
  - the stability of the compound (i.e. not chemically reactive)
  - the degradation to toxic compounds

[3] The IMAP (Inventory Multi-tiered Assessment and Prioritisation) programme is run by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS), to accelerate the assessment of human health and environmental impacts of unassessed industrial chemicals on The Australian Inventory of Chemical Substances (AICS; http://www.nicnas.gov.au/chemical-information/imap-assessments/imap-factsheets).

  - poorly soluble compounds (ecotoxicity and water solubility were compared automatically in Excel) and where co-solvents are used, how has this affected the result
  - complex substances where:
    - variation in the composition may affect ecotoxicity
    - the concentration of the substance may be difficult to define
    - impurities may be the source of the ecotoxicity
- endpoints used in determining the PNEC must not be greater than the chemical substance's water solubility, and
- ionisable chemicals.

Additionally, a manual check of the reactivity of the chemicals was conducted by identifying which chemicals had functional groups such as esters and amides, as these groups are susceptible to degradation by hydrolysis. However, in all cases, these chemicals were regarded as sufficiently stable for the duration of the test as these functional groups generally require either acid or base catalysis outside of the environmental pH range to proceed at an appreciable rate (with the exception of benzyl esters substituted with strong electron withdrawing groups such as NO_2 and Cl at the *p* position) (Morrison and Boyd 1983).

In addition to the scientific validity, a manual check of the data entry was also undertaken. Sources of error included CAS RN being split across rows, or Excel misinterpreting the CAS RN as dates and hence altering the CAS RN to form a valid date.

1.3.1.2 Modelled chemical data

The quality assurance of the modelled data was based on the limitations of the model described by Mayo-Bean et al. (2012a and 2012b). The major limitations are highlighted below.

- The modelling of surfactant chemicals (see discussion above).
- Chemicals that may have a special mode of action (e.g. herbicidal) but are not accounted for in the modelling.
- A chemical may be categorised into several chemical classes or sub-classes, with multiple ecotoxicity endpoints estimated. The following outlines how to choose the most appropriate value, when more than one endpoint is modelled for classes or sub-classes:
  - where there are multiple endpoints, conservatively the lowest endpoint may be used. Where possible, professional judgement using knowledge of environmental toxicology, organic chemistry, and statistics should be used to determine the most appropriate chemical class (Mayo-Bean et al. 2012b). A discussion on the chemicals categorised in multiple classes is provided below (see Section 1.9).
  - chemicals may be categorised into sub-classes. These sub-classes tend to give better consideration of all of the structural features of a molecule, but by their nature tend to have fewer chemicals in the training set. A check was conducted to determine whether any chemicals were categorised in a sub-class (see Table A.4).

- Chemicals with high molecular weights (> 1 000 g/mol) may not be adequately modelled.
- The solubility in water and n-octanol changes significantly for ionisable compounds depending on pH. Although KOWWIN adjusts Kow to pH 7, there are exceptions to this rule (US EPA 2000-2012). Therefore, these chemicals were further checked for quality.
- Chemicals for which there are no representative functional group(s) or other structural features in the training set.

1.3.2 Quality control (data outputs)

The choice of data critically affects the validity of the results produced by the model. Therefore, datasets must be chosen carefully as their quality may vary considerably. If there are several sources of data, they must be weighted and / or combined in appropriate mathematical ways (DoEE 2017b).

For several chemicals, there were multiple endpoints for the same study. Generally, all endpoint data were considered valid unless there was substantial evidence to consider otherwise. Consideration was given to the recording of the substance actually tested (e.g. whether the chemical is merely a solvent) and the study authors' notes into precisely what parameter was being tested. This was particularly pertinent for chronic fish data, for which the QSAR Toolbox contained significant quantities of information relating to matters other than direct toxicity of the chemical of interest to fish. If there were multiple endpoints for a trophic level, the lowest value was considered unless it was considered a potential outlier. Outliers was determined using expert judgement. Again, consideration was given to how the substance actually tested was recorded (e.g. was the chemical a solvent), control data, quality of test outcomes as noted by QSAR Toolbox, and test authors' notes. In addition, where there was doubt, the Grubb's test was used as the most appropriate test for judging whether a single data point was an outlier for normally distributed values (NIST/SEMATECH 2012 citing Grubb 1950)

When the LD50 values were reported as 100 mg/L, consideration was given to whether these are limit tests as prescribed by OECD TG 203 (OECD 1992a) and would be more accurately regarded as having a toxic concentration of ≥ 100 mg/L. Where values were reported as ranges rather than single points, the lowest value was used. Values reported as *less than* were not included in the analysis.

Where units were reported in mg/kg, the density of the solution was assumed to be 1 g/L (the same as pure water). This is considered reasonable based on 10 % w/w saline solutions having a density of 1.0688 g/mL (Aylward and Findlay 1974) and that most solutions were considerably more dilute than the saline solution. The lowest endpoint data points recorded in Table A.3 were considered outliers.

Table A.3 Quality assurance of study endpoints

CAS RN	Name	Value	Reference*	Reasons for rejection
64-17-5	Ethanol	42 mg/L	Fingas et al. (1995)	The toxicity data obtained related to a formulation which may contain other substances contributing to the toxicity. It was considered a significant outlier (Grubbs' test) when > 100 mg/L was excluded from the values

CAS RN	Name	Value	Reference*	Reasons for rejection
67-56-1	Methanol	290 mg/L	Kovriznych and Urbancikova (2001)	The test used to assess this substance's toxicity was designed to measure the effects on blastulae (larvae). It was also tested on a formulation which may contain other substances contributing to the toxicity
7783-20-2	Ammonium sulfate	0.068 mg/L	Rice and Bailey (1980)	QSAR does not typically provide reliable predictions of toxicity for ionisable substances without specifically modified models.

* *All references are cited in LMC (2012).*

1.4 QSAR data selection

The output data produced by QSAR models were quality checked. All of the assignments of chemical class were manually checked using professional judgement. None of the chemicals were considered to be misclassified or to have functional groups which are unlikely to be represented by the training set.

As previously discussed, the quality assurance of QSAR data focussed on complex molecules with many functional groups (item 3), high molecular weight compounds (item 4) and ionisable compounds (item 5). The chemicals listed in Table A.4 fell into one of these categories.

Table A.4 Quality assurance for QSAR modelled endpoints

CAS RN	Name	Reason for QA	Class (subclass) where appropriate*
52-51-7	1,3-Propanediol, 2-bromo-2-nitro-	Multiple classes (2 classes; 0 sub-classes)	Halo alcohols, nitro alcohols
CBI	Quaternary amine	Ionisable (QA)	-
141-43-5	2-amino-ethanol	Ionisable (QA)	-
2634-33-5	1,2-benzisothiazol-3(2h)-one	Multiple Classes (2 class, 0 sub-classes)	Isothiazolone, amide
6381-77-7	Sodium erythorbate;d-erythro-hex-2-enonic acid, .gamma.-lactone, monosodium salt;	Multiple classes (3 classes; 0 sub-classes), ionisable	Vinyl/Allyl Alcohols, Esters, Vinyl/Allyl Esters.
26172-55-4	3(2H)-isothiazolone, 5-chloro-2-methyl-	Multiple classes (2 classes, 0 sub-classes)	Isothiazolone, Vinyl/Allyl halides
64-02-8	Sodium edetate	Ionisable (QA)	-
CBI	Amine salt	Ionisable (QA)	-
127-09-3	Acetic acid, sodium salt	Ionisable (QA)	-
77-92-9	Citric acid	Ionisable (QA)	-

*The determination of whether the classification belonged to a class or sub-class was in accordance with US EPA (2012).

For the ionisable compounds, a manual check of the endpoints was conducted. Generally, salts of carboxylic acids are considered to have low ecotoxicity (> 100 mg/L) (Verschueren 1996) and low molecular weight (< 200 g/mol) tertiary amines are expected to have acute ecotoxicity values generally in the range of 1 to 100 mg/L (OECD 2012b). All of the ionisable chemicals manually checked had ecotoxicity values within the expected ranges.

Four chemicals were found to have multiple classes but none were categorised in the sub-classes. As a default, the lowest ecotoxicity value for the classes was considered first. This class was then assessed on the information contained in US EPA (2012) regarding the robustness of the training set of the chemicals in the class. Consideration was given to the number of data points including base toxicity if included.

The predicted ecotoxicity values for 1,3-propanediol, 2-bromo-2-nitro were considered. Both training sets for halo alcohols and nitro alcohols had limited data (≤ 3 data points) in the training sets. Therefore, the lowest value was used as a default.

Similarly, the predicted ecotoxicity values for 1,2-benzisothiazol-3(2h)-one were considered. Even though few data points existed in the training set for the isothiazolone class, the class definition was an exact match for the chemical. As the values for the isothiazolone class were also the lowest values, these were considered the most appropriate.

The predicted ecotoxicity values for 3(2h)-isothiazolone, 5-chloro-2-methyl- was considered in a similar fashion to 1,2-benzisothiazol-3(2h)-one. Again, the class definition was very similar to the chemical of interest. As the values for the isothiazolone class were also the lowest values, these were considered to be the most appropriate.

1.5 Data gaps

To conduct a risk assessment, the PNECs for aquatic, sediment and terrestrial species were sought. However, it was apparent that no study data existed for chemicals associated with coal seam gas for sediment and terrestrial species. There was also a paucity of study data for chronic effects on aquatic species.

Consideration was given to modelled data for earthworms, sediment dwelling organisms and chronic exposure of aquatic species using QSAR models from ECOSAR v1.1. However, based on log Kow, the applicability of QSAR models to terrestrial species appear to be less well-understood and less verified than for aquatic species. Additionally, for chronic effects on aquatic species, the QSAR models included extrapolations from acute study endpoints calculated by applying acute to chronic ratios (ACRs). However, these ratios do not take into account different modes of action under short- and long-term conditions and are also not fixed but instead are dependent on the log Kow of a chemical (Mayo-Bean et al. 2012a).

Due to these uncertainties, it was decided not to use values generated using QSAR models for sediment or terrestrial species, or for chronic aquatic ecotoxicity values.

1.6 Establishing PNECs

All endpoint values were converted to mg/L using standard values for molecular weight and / or density from Atkins (1986). Where the units were recorded as mg solute/kg solvent, a density of 1 g/cm^3 was assumed, precise to 1 significant figure. Where ranges of values or *greater than* a value were reported, the lowest value was used. Where values were reported as *less than* a certain value, these were not included in the analysis, as the value cannot be relied on.

A PNEC is calculated using toxicity test data such as LC50, EC50, other L(E)Cx values, NOEC (no observed effect concentration) and LOEC (lowest observed effect concentration). MATC (maximum allowable toxicant concentration, calculated as MATC = (NOEC x LOEC)1/2) is also used in effects assessment (OECD 2002c).

Derivation of a PNEC within a deterministic assessment framework commonly relies on using assessment factors. Assessment factors reflect the following uncertainties inherent in most datasets, and the extrapolations that can be required:

- intra-species and inter-species variations
- the extrapolation of short-term toxicity towards long-term toxicity
- the extrapolation of laboratory results towards the field (OECD 2002c; EPHC 2009).

Assessment factors are used to adjust the effect concentration and to estimate a PNEC. They should be applied with care to acute data for substances which are suspected of having a specific mode of action, have a high log Kow or which significantly bioaccumulate. As well, they should be applied with care to data on chemicals of limited solubility and no observed toxicity, such as some inorganic salts or 'totally' insoluble chemicals such as polystyrene or silicon.

In the following paragraphs, assessment factors to be used in estimating PNEC from expected available datasets are proposed (OECD 2002c; EPHC 2009).

1.7 Assessment factors

The assessment factor method is most commonly used to derive a PNEC when only acute toxicity data or limited chronic toxicity data are available, as was the case in this assessment (EPHC 2009). In general, the selection of the assessment factor followed the principles outlined in the OECD method. However, in situations where no clear guidance was given, particularly concerning the use of measured or modelled data and the use of data from published studies, some variations and / or refinements to the OECD method were applied.

As stipulated in the OECD method, the use of field (measured) or modelled ecosystem data in the assessment can be determined on a case-by-case basis. On this basis, the general rules used to select assessment factors in this study were as follows:

- An assessment factor of 1 000 was used if a single measured or modelled acute endpoint with no reference to published data was available, consistent with the relevant OECD method for the availability of limited data i.e. an acute EC/LC50 value with no evidence provided for its deriviation was considered to justify a reduction in this value by 100.
- An assessment factor of 100 was used in the following situations:
  - if a single measured acute endpoint with a reference to published data was available. This is consistent with the OECD method for the availability of limited data with evidence to justify reduction in the assessment factor to 100
  - if at least three measured acute endpoints from three trophic levels with or without references to published data were available. This is consistent with the OECD method for the availability of at least one EC/LC50 from each trophic level
  - if at least one modelled acute endpoint was available from each relevant trophic level. This is consistent with the OECD method for the availability of at least one EC/LC50 from each trophic level

  - if the lowest measured chronic endpoint for fish and / or *Daphnia* was available. This is consistent with the OECD method for the availability of one NOEC for either fish or *Daphnia*.

- An assessment factor of 50 was used in one case where an endpoint was inferred from an overall PNEC and the endpoint type was classed as sub-chronic.
- An assessment factor of 10 was used if the lowest measured chronic endpoint for fish and / or *Daphnia* was available, if three modelled acute endpoints were available for each trophic level and at least one measured acute endpoint with or without references to published data was also available. This was not consistent with the OECD method but was deemed to be equivalent to at least three NOECs from three species / trophic levels.

Moreover, because the selection of endpoints was conducted purely on the ecotoxicity of the chemicals, with no consideration given to a chemical's physico-chemical properties and interaction with environmental mediums, the following rules were also applied in the assessment of whether data was appropriate for inclusion in this report:

- If no reference to published data was available, a modelled acute endpoint was selected over a measured acute endpoint.
- If a reference to published data was available, a measured acute endpoint was selected over modelled acute endpoints.
- Preference was given to chronic data because it is considered that uncertainty is lower in chronic data (Guidance Document on Aquatic Ecotoxicology, 2001 EEC).

1.8 Resulting PNECs

The data sets used to calculate the PNEC values include documentation which outline the selection of endpoints and assessment factor values for each chemical. In cases where the selection of the assessment factor did not completely align with the OECD method, expert judgement was used to evaluate the data and refine the selection criteria used for this assessment on a case-by-case basis.

The final ecotoxicity endpoints and PNEC values for the chemicals and their assessment factors are summarised in Table A.5 and Table A.6 (drilling chemicals), and Table A.7 and Table A.8 (hydraulic fracturing chemicals).

1.9 Final quality control

As a final means of quality control, the output data from all measured and modelled endpoint values were compared to the published values (where available) including PNECs, as these had already been peer-reviewed. In many cases, the output values from QSAR Toolbox and ECOSAR concurred with the published data. Unless otherwise indicated, published data was given preference as it is based on peer-reviewed, detailed studies rather than summary information on endpoints and modelled data. Table A.9 presents a summary of this work.

Table A.5 Calculated PNEC values (Acute) of the drilling chemicals within different trophic levels and exposure scenarios

Drilling		Effect type:	ACUTE																
		Trophic level:	1. Primary producers			2. Primary consumers			3. Secondary consumers			Lowest acute endpoint							
		Indicator species:	Algae			Daphnia			Fish			Derived endpoint				Published data available?			
Ref No.	*CAS RN*	*Chemical name*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Algae) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Daphnia) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Fish) mg/L*	*No. of acute endpoint species*	*Lowest acute endpoint species*	*Lowest acute endpoint mg/L*	*Measured or modelled?*	*Published data - endpoint mg/L?*	*Test details*	*Reference*	*Lowest acute endpoint mg/L*
1	CBI	2-Ethylhexanol heavies	0	14.093	14.093	0	14.307	14.307	28.2	23.55	28.2	3	Algae	14.093	Modelled				14.1
2	107222	Ethanedial	0	5.815	5.815	0	38.047	38.047	215	21.574	215	3	Algae	5.815	Modelled	215	96-h LC50 (Fish)	OECD (2003a)	215
3	111308	Pentanedial	0	2.871	2.871	0	16.35	16.35	3.5	11.233	3.5	3	Algae	2.871	Modelled	0.9	96-h EC50 (Algae)	OECD (2001b)	0.90
4	11138662	Xanthan gum	0	-	-	0	-	-	420	-	420	1	Fish	420	Measured				420
5	1305620	Calcium hydroxide (Ca(OH)2)	0	-	-	0	-	-	356	-	356	1	Fish	356	Measured				356
6	1310732	Sodium hydroxide (NaOH)	0	-	-	0	-	-	196	-	196	1	Fish	196	Measured				196
7	144558	Carbonic acid, monosodium salt	0	-	-	0	-	-	8250	-	8250	1	Fish	8250	Measured				8250
8	CBI	Ester alcohol	0	5.141	5.141	0	14.146	14.146	0	7.572	7.572	3	Algae	5.141	Modelled	18.4	72-h EC50 (Algae)	OECD (2002a)	18.40
9	497198	Carbonic acid, disodium salt	0	-	-	0	-	-	300	-	300	1	Fish	300	Measured				300
10	64175	Ethanol	0	485.795	485.795	0	1476.944	1476.944	10257	3169.759	10257	3	Algae	485.795	Modelled	1000	96-h EC50 (Algae)	OECD (2005b)	1000
11	64742478	Distillates, petroleum, hydrotreated light	0	0.069	0.069	0	0.018	0.018	2.2	0.022	2.2	3	Daphnia	0.02	Modelled				0.02
12	67561	Methanol	0	739.102	739.102	0	2710.44	2710.44	15029	6086.885	15029	3	Algae	739.102	Modelled	15400	96-h LC50 (Fish)	Dept. Env. (2013n) in LMC (2012)	15400
13	67630	2-Propanol	0	325.707	325.707	0	844.305	844.305	6550	1743.475	6550	3	Algae	325.71	Modelled		No superior information	OECD (2002b)	325.71
14	CBI	Organic sulfate	0	-	-	0	-	-	0	-	-	0		-	-	0.74			0.74
15	CBI	Organic acid salt	0	13.016	13.016	0	3357.137	3357.137	0	3357.137	3357.137	3	Algae	13.02	Modelled				13.02

Drilling		Effect type:	ACUTE															
		Trophic level:	1. Primary producers			2. Primary consumers			3. Secondary consumers			Lowest acute endpoint						
		Indicator species:	Algae			Daphnia			Fish			Derived endpoint				Published data available?			
Ref No.	*CAS RN*	*Chemical name*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Algae) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Daphnia) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Fish) mg/L*	*No. of acute endpoint species*	*Lowest acute endpoint species*	*Lowest acute endpoint mg/L*	*Measured or modelled?*	*Published data - endpoint mg/L?*	*Test details*	*Reference*	*Lowest acute endpoint mg/L*
16	7447407	Potassium chloride (KCl)	0	-	-	0	-	-	880	-	880	1	Fish	880	Measured				880
17	7757837	Sulfurous acid, disodium salt	0	-	-	118	-	118	170	-	170	2	Daphnia	118	Measured	118	48-h EC50 (Daphnia)	OECD (2009b)	118
18	7758169	Diphosphoric acid, disodium salt	63	-	63	0	-	-	0	-	-	1	Algae	63	Measured				63
19	7778805	Sulfuric acid, dipotassium salt	0	-	-	0	-	-	680	-	680	1	Fish	680	Measured				680
20	77929	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	0	233000	233000	0	1270000	1270000	0	3140000	3140000	3	Algae	233000	Modelled	98	EC50 (Daphnia) - no time specified, but similar to 24-h EC50	OECD (2004b)	98
21	CBI	Polymer with substituted alkylacrylamide salt		0.397		0	161.006	161.006	34.8	64.917	34.8	3	Algae	0.40	Modelled				0.40
22	9000300	Guar gum	0	-	-	0	-	-	218	-	218	1	Fish	218	Measured				218
23	CBI	Polymer	0	5.2E-09	5.2E-09	0	2.1E-11	2.1E-11	0	9.06E-12	9.06E-12	3	Fish	9.06E-12	Modelled				9.06E-12

Table A.6 Calculated PNEC values (Chronic and Overal Aquatic Ecotoxicity) of the drilling chemicals within different trophic levels and exposure scenarios

Drilling		**Effect type:**	**CHRONIC**						**OVERALL AQUATIC ECOTOXICITY**				
		Trophic level:	**Chronic endpoint**						**Final reported values**				
		Indicator species:	**Parameters**		**Published data available?**								
Ref No.	***CAS RN***	***Chemical name***	***Chronic endpoint (Daphnia) mg/L***	***Chronic endpoint (Fish) mg/L***	***Published data - endpoint mg/L?***	***Test details***	***Reference***	***Final chronic endpoint mg/L***	***Ecotoxicity endpoint value mg/L***	***Measured or modelled?***	***Ecotoxity endpoint type (species)***	***Assessment factor (AF)***	***PNEC mg/L***
1	CBI	2-Ethylhexanol heavies	-	-				-	14.1	Modelled	Acute (Algae)	100	0.141
2	107222	Ethanedial	-	-				-	215	Measured	Acute (Fish)	100	2.15
3	111308	Pentanedial	2.1	-	2.1	NOEC 21 day Daphnia	Unknown	2.1	2.1	Measured	Chronic (Daphnia)	10	0.210
4	11138662	Xanthan gum	-	-				-	420	Measured	Acute (Fish)	1000	0.420
5	1305620	Calcium hydroxide (Ca(OH)2)	-	-				-	356	Measured	Acute (Fish)	1000	0.356
6	1310732	Sodium hydroxide (NaOH)	240	-				240	240	Measured	Chronic (Daphnia)	100	2.40
7	144558	Carbonic acid, monosodium salt	576	-				576	576	Measured	Chronic (Daphnia)	100	5.76
8	CBI	Ester alcohol	-	-				-	18.4	Measured	Acute (Algae)	100	0.184
9	497198	Carbonic acid, disodium salt	424	-				424	424	Measured	Chronic (Daphnia)	100	4.24
10	64175	Ethanol	7800	-				7800	7800	Measured	Chronic (Daphnia)	10	780
11	64742478	Distillates, petroleum, hydrotreated light	-	-				-	0.018	Modelled	Acute (Daphnia)	100	1.80E-04
12	67561	Methanol	32000	-				32000	32000	Measured	Chronic (Daphnia)	10	3.20E+03
13	67630	2-Propanol	5000	-				5000	5000	Measured	Chronic (Daphnia)	10	500
14	CBI	Organic sulfate	0.37	-	0.37			0.37	0.37	Measured	Chronic (Daphnia)	10	0.0370
15	CBI	Organic acid salt	-	-				-	13	Modelled	Acute (Algae)	100	0.130
16	7447407	Potassium chloride (KCl)	373	-				373	373	Measured	Chronic (Daphnia)	100	3.73
17	7757837	Sulfurous acid, disodium salt	3780	-				3780	3780	Measured	Chronic (Daphnia)	100	37.8
18	7758169	Diphosphoric acid, disodium salt	-	-				-	63	Measured	Acute (Algae)	1000	0.0630
19	7778805	Sulfuric acid, dipotassium salt	-	-				-	680	Measured	Acute (Fish)	1000	0.680

Drilling		Effect type:	CHRONIC						OVERALL AQUATIC ECOTOXICITY				
		Trophic level:	Chronic endpoint						Final reported values				
		Indicator species:	Parameters		Published data available?								
Ref No.	***CAS RN***	***Chemical name***	***Chronic endpoint (Daphnia) mg/L***	***Chronic endpoint (Fish) mg/L***	***Published data - endpoint mg/L?***	***Test details***	***Reference***	***Final chronic endpoint mg/L***	***Ecotoxicity endpoint value mg/L***	***Measured or modelled?***	***Ecotoxity endpoint type (species)***	***Assessment factor (AF)***	***PNEC mg/L***
20	77929	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	153	-				153	153	Measured	Chronic (Daphnia)	10	15.3
21	CBI	Polymer with substituted alkylacrylamide salt	-	-				-	0.397	Modelled	Acute (Algae)	100	3.97E-03
22	9000300	Guar gum	-	-				-	218	Measured	Acute (Fish)	1000	0.218
23	CBI	Polymer	-	-				-	9.06E-12	Modelled	Acute (Fish)	100	9.06E-14

Table A.7 Calculated PNEC values (Acute) of the hydraulic fracturing chemicals within different trophic levels and exposure scenarios

Hydraulic fracturing		**Effect type:**	**ACUTE**																
		Trophic level:	**1. Primary producers**			**2. Primary consumers**			**3. Secondary consumers**			**Lowest acute endpoint**							
		Indicator species:	**Algae**			**Daphnia**			**Fish**			**Derived endpoint**				**Published data available?**			
Ref No.	***CAS RN***	***Chemical name***	***Measured endpoint mg/L***	***Modelled endpoint (QSAR) mg/L***	***Acute endpoint (Algae) mg/L***	***Measured endpoint mg/L***	***Modelled endpoint (QSAR) mg/L***	***Acute endpoint (Daphnia) mg/L***	***Measured endpoint mg/L***	***Modelled endpoint (QSAR) mg/L***	***Acute endpoint (Fish) mg/L***	***No. of acute endpoint species***	***Lowest acute endpoint species***	***Lowest acute endpoint mg/L***	***Measured or modelled?***	***Published data - endpoint mg/L?***	***Test details***	***Reference***	***Lowest acute endpoint mg/L***
1	10043353	Boric acid (H_3BO_3)	0	-	-	0	-	-	447	-	447	1	Fish	447	Measured				447
2	10043524	Calcium chloride ($CaCl_2$)	0	-	-	0	-	-	2110	-	2110	1	Fish	2110	Measured				2110
3	107211	1,2-Ethanediol	0	3536.208	3536.208	0	16103.915	16103.92	8050	38109.7	8050	3	Algae	3536.208	Modelled				3536
4	108101	2-Pentanone, 4-methyl-	0	131.743	131.743	0	243.279	243.279	505	462.803	505	3	Algae	131.743	Modelled				131.743
5	111762	Ethanol, 2-butoxy-	0	403.305	403.305	0	935.818	935.818	983	1881.356	983	3	Algae	403.305	Modelled	911	EC50 Algae	OECD 2006	911
6	111900	Ethanol, 2-(2-ethoxyethoxy)-	0	3393.091	3393.091	0	12720.301	12720.3	9650	28718.81	9650	3	Algae	3393.091	Modelled	> 500	Modelled	OECD (2007c)	3393
7	1310732	Sodium hydroxide (Na(OH))	0	-	-	0	-	-	196	-	196	1	Fish	196	Measured				196
8	141435	Ethanol, 2-amino-	0	411.043	411.043	97	217.035	97	150	2771.054	150	3	Daphnia	97	Measured				97
9	144558	Carbonic acid, monosodium salt	0	-	-	0	-	-	8250	-	8250	1	Fish	8250	Measured				-
10	26172554	3(2H)-Isothiazolone, 5-chloro-2-methyl-	0.062	0.455	0.062	0	3.486	3.486	0.19	2.758	0.19	3	Algae	0.062	Measured				0.062
11	2634335	1,2-Benzisothiazol-3(2H)-one	0	0.283	0.283	0	1.175	1.175	1.6	0.881	1.6	3	Algae	0.283	Modelled				0.283
12	2682204	3-Isothiazolone, 2-methyl-	0	0.448	0.448	0	4.667	4.667	0.07	3.792	0.07	3	Fish	0.07	Measured				0.07
13	497198	Carbonic acid, disodium salt	0	-	-	0	-	-	300	-	300	1	Fish	300	Measured				300
14	52517	1,3-Propanediol, 2-bromo-2-nitro-	0	0.109	0.109	0	3514.984	3514.984	20	777.831	20	3	Algae	0.109	Modelled				0.109
15	55566308	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	0	4.43E+17	4.43E+17	0	3.06E+21	3.06E+21	94	4.26E+22	94	3	Fish	94	Measured				94

Hydraulic fracturing		Effect type:	ACUTE																
		Trophic level:	1. Primary producers			2. Primary consumers			3. Secondary consumers			Lowest acute endpoint							
		Indicator species:	Algae			Daphnia			Fish			Derived endpoint				Published data available?			
Ref No.	*CAS RN*	*Chemical name*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Algae) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Daphnia) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Fish) mg/L*	*No. of acute endpoint species*	*Lowest acute endpoint species*	*Lowest acute endpoint mg/L*	*Measured or modelled?*	*Published data - endpoint mg/L?*	*Test details*	*Reference*	*Lowest acute endpoint mg/L*
16	56815	1,2,3-Propanetriol	0	10797.66	10797.661	0	58451.754	58451.75	68094	144000	68094	3	Algae	10797.661	Modelled	> 2900	Unknown	OECD (2005a)	10798
17	CBI	Amine salt	0.19	27.134	0.19	0	20.944	20.944	0	220.707	220.707	3	Algae	0.19	Measured				0.19
18	CBI	Inner salt of alkyl amines	0	211.236	211.236	0	17977.443	17977.44	0	8916.546	8916.546	3	Algae	211.236	Modelled				211.236
19	CBI	Ethoxylated fatty acid (1)	0	0.007	0.007	0	2.595	2.595	0	2.595	2.595	3	Algae	0.007	Modelled	2.2	Unknown	Unknown	2.2
20	CBI	Ethoxylated fatty acid (2)	0	6.68E-09	6.68E-09	0	1.62E-07	1.62E-07	0	3.77E-07	3.77E-07	3	Algae	6.68E-09	Modelled	5	Unknown	Unknown	5
21	CBI	Ethoxylated fatty acid (3)	0	7.057	7.057	0	20.095	20.095	0	11.007	11.007	3	Algae	7.057	Modelled				7.057
22	6381777	D-Erythro-hex-2-enonic acid, .gamma.-lactone, monosodium salt	0	0	0	0	0	0	0	0	0	0	0	0	-	1020	L-ascorbic acid	NICNAS 2013	1020
23	6410419	2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-	0	0.00181	0.00181	0	0.00139	0.00139	0	0.017	0.017	3	Daphnia	0.00139	Modelled				0.00139
24	64175	Ethanol	0	485.795	485.795	0	1476.944	1476.944	10257	3169.759	10257	3	Algae	485.795	Modelled	1000	96-h EC50 (Algae)	OECD (2005b)	1000
25	64197	Acetic acid	0	-	-	0	-	-	75	-	75	1	Fish	75	Measured	32	EC50 (Daphnia)	Dept. Env. (2013a) in LMC 2012	75
26	67561	Methanol	0	739.102	739.102	0	2710.44	2710.44	15029	6086.885	15029	3	Algae	739.102	Modelled	15400	96-h LC50 (Fish)	Dept. Env. (2013n) in LMC 2012	15400
27	67630	2-Propanol	0	325.707	325.707	0	844.305	844.305	6550	1743.475	6550	3	Algae	325.707	Modelled	?	No superior	OECD (2002b)	325.707

Hydraulic fracturing		Effect type:	ACUTE																
		Trophic level:	1. Primary producers			2. Primary consumers			3. Secondary consumers			Lowest acute endpoint							
		Indicator species:	Algae			Daphnia			Fish			Derived endpoint				Published data available?			
Ref No.	*CAS RN*	*Chemical name*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Algae) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Daphnia) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Fish) mg/L*	*No. of acute endpoint species*	*Lowest acute endpoint species*	*Lowest acute endpoint mg/L*	*Measured or modelled?*	*Published data - endpoint mg/L?*	*Test details*	*Reference*	*Lowest acute endpoint mg/L*
																	information		
28	68187177	Sulfuric acid, mono-C_{6-10}-alkyl esters, ammonium salts	0	186.723	186.723	0	308.362	308.362	0	570.977	570.977	3	Algae	186.723	Modelled	33	Unknown	Unknown	33
29	68439452	Alcohols, C_{6-12}, ethoxylated	0	300.461	300.461	0	500.762	500.762	0	929.291	929.291	3	Algae	300.461	Modelled	4.87	Inferred from overall PNEC - fish	Unknown	4.87
30	68647723	Terpenes and terpenoids, orange oil	0	0.522	0.522	0	0.238	0.238	0	0.323	0.323	3	Daphnia	0.238	Modelled				0.238
31	7447407	Potassium chloride (KCl)	0	-	-	0	-	-	880	-	880	1	Fish	880	Measured				880
32	CBI	Quaternary amine	0	27.134	27.134	0	20.944	20.944	0	220.707	220.707	3	Daphnia	20.944	Modelled				20.944
33	75570	Methanaminium, N,N,N-trimethyl-, chloride	0	490000	490000	0	6960000	6960000	462	21700000	462	3	Fish	462	Measured				462
34	7647010	Hydrochloric acid	0.492	-	0.492	0.492	-	0.492	4.92	-	4.92	3	Daphnia	0.492	Measured				0.492
35	7647145	Sodium chloride (NaCl)	0	-	-	0	-	-	1290	-	1290	1	Fish	1290	Measured				1290
36	7681529	Hypochlorous acid, sodium salt	0	-	-	0	-	-	0.023	-	0.023	1	Fish	0.023	Measured				0.023
37	7727540	Peroxydisulfuric acid ($(((HO)S(O)_2)_2O_2$), diammonium salt	0	-	-	0	-	-	0	-	-	0	-	-	-	92	48-h EC50 (Daphnia)	OECD (2006a)	92
38	7757826	Sulfuric acid, disodium salt	3360	-	3360	4580	-	4580	3040	-	3040	3	Fish	3040	Measured	1900	120-h EC50	OECD (2006b)	3040
39	7757837	Sulfurous acid, disodium salt	0	-	-	118	-	118	170	-	170	2	Daphnia	118	Measured	118	48-h EC50 (Daphnia)	OECD (2006b)	118
40	7758192	Chlorous acid, sodium salt	0.904	-	0.904	0	-	0	203	-	203	2	Algae	0.904	Measured	0.063	48-h EC50 (Daphnia)	OECD (2006c)	0.063

Hydraulic fracturing		Effect type:	ACUTE															
		Trophic level:	1. Primary producers			2. Primary consumers			3. Secondary consumers			Lowest acute endpoint						
		Indicator species:	Algae			Daphnia			Fish			Derived endpoint				Published data available?			
Ref No.	*CAS RN*	*Chemical name*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Algae) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Daphnia) mg/L*	*Measured endpoint mg/L*	*Modelled endpoint (QSAR) mg/L*	*Acute endpoint (Fish) mg/L*	*No. of acute endpoint species*	*Lowest acute endpoint species*	*Lowest acute endpoint mg/L*	*Measured or modelled?*	*Published data - endpoint mg/L?*	*Test details*	*Reference*	*Lowest acute endpoint mg/L*
41	7775271	Peroxydisulfuric acid ($(HO)S(O)_2)_2O_2$), disodium salt	0	-	-	140	16135.55	140	-	-	-	1	Daphnia	140	Measured				140
42	7783202	Sulfuric acid, diammonium salt	0	-	-	0	-	-	6.6	-	6.6	1	Fish	6.6	Measured	173	Unknown	OECD (2006b)	173
43	7786303	Magnesium chloride ($MgCl_2$)	0	-	-	0	-	-	2120	-	2120	1	Fish	2120	Measured				2120
44	77929	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	0	233000	233000	0	1270000	1270000	0	3140000	3140000	3	Algae	233000	Modelled	98	EC50 (Daphnia) - no time specified, but similar to 24-h EC50	OECD (2004b)	98
45	81741288	Phosphonium, tributyltetradecyl-, chloride	-	-	-	0	16.788	16.788	0	1059.253	1059.253	2	Daphnia	16.788	Modelled				16.788
46	9000300	Guar gum	0	-	-	0	-	-	218	-	218	1	Fish	218	Measured				218

Table A.8 Calculated PNEC values (Chronic and Overall Aquatic Ecotoxicity) of the hydraulic fracturing chemicals

Drilling		**Effect type:**	**CHRONIC**						**OVERALL AQUATIC ECOTOXICITY**				
		Trophic level:	**Chronic endpoint**						**Final reported values**				
		Indicator species:	**Parameters**		**Published data available?**								
Ref No.	***CAS RN***	***Chemical name***	***Chronic endpoint (Daphnia) mg/L***	***Chronic endpoint (Fish) mg/L***	***Published data - endpoint mg/L?***	***Test details***	***Reference***	***Final chronic endpoint mg/L***	***Ecotoxicity endpoint value mg/L***	***Measured or modelled?***	***Ecotoxity endpoint type (species)***	***Assessment factor (AF)***	***PNEC mg/L***
1	10043353	Boric acid (H_3BO_3)	6	2.1				2.1	2.1	Measured	Chronic (Fish)	100	0.0210
2	10043524	Calcium chloride ($CaCl_2$)	920	-				920	920	Measured	Chronic (Daphnia)	100	9.20
3	107211	1,2-Ethanediol	100	-	100	21-d NOEC (Daphnia)	OECD (2009a)	100	100	Measured	Chronic (Daphnia)	10	10.0
4	108101	2-Pentanone, 4-methyl-	7.8	246	7.8	21-d NOEC (Daphnia)	OECD (2011b)	7.8	7.8	Measured	Chronic (Daphnia)	10	0.780
5	111762	Ethanol, 2-butoxy-	1000	-				1000	1000	Measured	Chronic (Daphnia)	10	100
6	111900	Ethanol, 2-(2-ethoxyethoxy)-	-	-				-	3393	Modelled	Acute (Algae)	100	33.9
7	1310732	Sodium hydroxide (Na(OH))	240	-				240	240	Measured	Chronic (Daphnia)	100	2.40
8	141435	Ethanol, 2-amino-	0.85	-	0.85			0.85	0.85	Measured	Chronic (Daphnia)	10	0.0850
9	144558	Carbonic acid, monosodium salt	576	-				576	576	Measured	Chronic (Daphnia)	100	5.76
10	26172554	3(2H)-Isothiazolone, 5-chloro-2-methyl-	-	-				-	0.062	Measured	Acute (Algae)	100	6.20E-04
11	2634335	1,2-Benzisothiazol-3(2H)-one	-	-				-	0.28	Modelled	Acute (Algae)	100	2.80E-03
12	2682204	3-Isothiazolone, 2-methyl-	-	-				-	0.07	Measured	Acute (Fish)	100	7.00E-04
13	497198	Carbonic acid, disodium salt	424	-				424	424	Measured	Chronic (Daphnia)	100	4.24
14	52517	1,3-Propanediol, 2-bromo-2-nitro-	-	-				-	0.11	Modelled	Acute (Algae)	100	1.10E-03
15	55566308	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	-	-				-	94	Measured	Acute (Fish)	100	0.940
16	56815	1,2,3-Propanetriol	-	-				-	10798	Modelled	Acute (Algae)	100	107.98
17	CBI	Amine salt	-	-				-	0.19	Measured	Acute (Algae)	100	1.90E-03
18	CBI	Inner salt of alkyl amines	-	-				-	211	Modelled	Acute (Algae)	100	2.11
19	CBI	Ethoxylated fatty acid (1)	-	-				-	2.2	Measured	Acute (Algae)	100	2.20E-02

Drilling		Effect type:	CHRONIC						OVERALL AQUATIC ECOTOXICITY				
		Trophic level:	Chronic endpoint						Final reported values				
		Indicator species:	Parameters		Published data available?								
Ref No.	***CAS RN***	***Chemical name***	***Chronic endpoint (Daphnia) mg/L***	***Chronic endpoint (Fish) mg/L***	***Published data - endpoint mg/L?***	***Test details***	***Reference***	***Final chronic endpoint mg/L***	***Ecotoxicity endpoint value mg/L***	***Measured or modelled?***	***Ecotoxity endpoint type (species)***	***Assessment factor (AF)***	***PNEC mg/L***
20	CBI	Ethoxylated fatty acid (2)	-	-				-	5	Measured	Acute (Daphnia)	100	0.0500
21	CBI	Ethoxylated fatty acid (3)	-	-				-	7.1	Modelled	Acute (Algae)	100	7.10E-02
22	6381777	D-Erythro-hex-2-enonic acid, .gamma.-lactone, monosodium salt	-	-				-	1020	Measured	Acute (Algae)	100	10.2
23	6410419	2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-	-	-				-	0.0014	Modelled	Acute (Daphnia)	100	1.40E-05
24	64175	Ethanol	7800	-				7800	7800	Measured	Chronic (Daphnia)	10	780
25	64197	Acetic acid	150	-				150	150	Measured	Chronic (Daphnia)	10	15.0
26	67561	Methanol	32000	-				32000	32000	Measured	Chronic (Daphnia)	10	3200
27	67630	2-Propanol	5000	-				5000	5000	Measured	Chronic (Daphnia)	10	500
28	68187177	Sulfuric acid, mono-C_{6-10}-alkyl esters, ammonium salts	-	-				-	33	Measured	Acute (Daphnia)	100	0.330
29	68439452	Alcohols, C_{6-12}, ethoxylated	-	-				-	4.87	Measured	Sub-chronic (Fish)	50	0.0974
30	68647723	Terpenes and terpenoids, orange oil	-	-				-	0.24	Modelled	Acute (Daphnia)	100	2.40E-03
31	7447407	Potassium chloride (KCl)	373	-				373	373	Measured	Chronic (Daphnia)	100	3.73
32	CBI	Quaternary amine	-	-				-	20.9	Modelled	Acute (Daphnia)	100	0.209
33	75570	Methanaminium, N,N,N-trimethyl-, chloride	-	-				-	462	Measured	Acute (Fish)	100	4.62
34	7647010	Hydrochloric acid	62	-				62	62	Measured	Chronic (Daphnia)	10	6.20
35	7647145	Sodium chloride (NaCl)	314	-				314	314	Measured	Chronic (Daphnia)	100	3.14
36	7681529	Hypochlorous acid, sodium salt	-	-				-	0.023	Measured	Acute (Fish)	1000	2.30E-05
37	7727540	Peroxydisulfuric acid ($(HO)S(O)_2)_2O_2$), diammonium salt	-	-				-	92	Measured	Acute (Daphnia)	100	0.920

Drilling		Effect type:	CHRONIC						OVERALL AQUATIC ECOTOXICITY				
		Trophic level:	Chronic endpoint						Final reported values				
		Indicator species:	Parameters		Published data available?								
Ref No.	***CAS RN***	***Chemical name***	***Chronic endpoint (Daphnia) mg/L***	***Chronic endpoint (Fish) mg/L***	***Published data - endpoint mg/L?***	***Test details***	***Reference***	***Final chronic endpoint mg/L***	***Ecotoxicity endpoint value mg/L***	***Measured or modelled?***	***Ecotoxity endpoint type (species)***	***Assessment factor (AF)***	***PNEC mg/L***
38	7757826	Sulfuric acid, disodium salt	653	-				653	653	Measured	Chronic (Daphnia)	10	65.3
39	7757837	Sulfurous acid, disodium salt	3780	-				3780	3780	Measured	Chronic (Daphnia)	100	37.8
40	7758192	Chlorous acid, sodium salt	-	-				-	0.063	Measured	Acute (Daphnia)	100	6.30E-04
41	7775271	Peroxydisulfuric acid ($(HO)S(O)_2)_2O_2$), disodium salt	10	-				10	10	Measured	Chronic (Daphnia)	100	0.100
42	7783202	Sulfuric acid, diammonium salt	106	-	11	61-d NOEC (Fish)	OECD (2006c)	11	11	Measured	Chronic (Fish)	100	0.110
43	7786303	Magnesium chloride ($MgCl_2$)	-	-				-	2120	Measured	Acute (Fish)	1000	2.12
44	77929	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	153	-				153	153	Measured	Chronic (Daphnia)	10	15.3
45	81741288	Phosphonium, tributyltetradecyl-, chloride	-	-				-	16.8	Modelled	Acute (Daphnia)	1000	0.0168
46	9000300	Guar gum	-	-				-	218	Measured	Acute (Fish) (Daphnia)	1000	0.218

Table A.9 Comparison between derived and published ecotoxicity endpoints

CAS RN	Chemical name	Derived endpoint(s)	Published data	Reference	Selected endpoint
107-21-1	1,2-Ethanediol	100 mg/L 21-d NOEC Daphnia	100 mg/L 21-d NOEC Daphnia	OECD (2009a)	100 mg/L
107-22-2	Ethanedial	5.8 mg/L QSAR value for acute algae; 215 mg/L 96 h fish	215 mg/L 96 h-LC50 fish	OECD (2003a)	215 mg/L
108-10-1	2-Pentanone, 4-methyl-	7.8 mg/L 21-d NOEC Daphnia	7.8 mg/L 21-d NOEC Daphnia	OECD (2011b)	7.8 mg/L
111-30-8	Pentanedial	2.87 mg/L QSAR value for acute algae	0.9 mg/L 96 h-EC50 algae	OECD (2001b)	2.1 mg/L chronic Daphnia***
111-76-2	Ethanol, 2-butoxy-	403 mg/L QSAR value for acute algae	911 mg/L 96 h-EC50 algae	OECD (2007b)	1000 mg/L chronic Daphnia***
111-90-0	Ethanol, 2-(2-ethoxyethoxy)-	3393 mg/L QSAR value for acute algae	> 500 mg/L, estimated	OECD (2007c)	3393 mg/L
CBI	Ester alcohol	5.14 mg/L QSAR value for acute algae	18.4 mg/L EC50 72 h algae	OECD (2002a)	18.4 mg/L
56-81-5	1,2,3-Propanetriol	10798 mg/L QSAR value for acute algae	> 2900 mg/L	OECD (2005a)	10798 mg/L
64-17-5	Ethanol	486 mg/L QSAR value for acute algae	1000 mg/L EC50 96 h algae	OECD (2005b)	7800 mg/L chronic Daphnia***
64-19-7	Acetic acid	75 mg/L 96 h fish	32 mg/L	LMC (2012)	150 mg/L chronic Daphnia***
67-56-1	Methanol	739 mg/L QSAR value for acute algae; 15029 mg/L 96 h fish	15400 mg/L 96 h-LC50 fish	LMC (2012)	32000 mg/L chronic Daphnia***
67-63-0	2-Propanol	326 mg/L QSAR value for acute algae	No Additional information	OECD (2002b)	5000 mg/L chronic Daphnia***
7727-54-0	Peroxydisulfuric acid, diammonium salt	No value determined	92 mg/L EC50 48 h Daphnia	OECD (2006a)	92 mg/L
7757-82-6	Sulfuric acid, disodium salt	3 040 mg/L 96 h-LC50 fish	1900 mg/L EC50 120 h	OECD (2006b)	653 mg/L chronic Daphnia***
7758-19-2	Chlorous acid, sodium salt	0.904 mg/L 96 h algae	0.063 mg/L EC50 48 h Daphnia	OECD (2009c)	0.063 mg/L
7783-20-2	Sulfuric acid, diammonium salt	6.6 mg/L 96 h-LC50 fish	11 mg/L NOEC 61 day chronic	OECD (2006c)	11 mg/L
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	233 000 mg/L 96 h algae	98 mg/L* EC50 Daphnia, time not specified but the value is similar to the 24 h EC50	OECD (2004b)	153 mg/L chronic Daphnia***

** Unbuffered – this is expected to represent the bounding estimate where the environmental water has limited capacity to neutralise 1,2,3-Propanetricarboxylic acid, 2-hydroxy- (citric acid). *** This value is selected as it was considered more representative and protective.*

1.10 Physico-chemical data

To predict the exposure of chemicals associated with coal seam gas to the environment, the chemical fate pathways which may result in loss of chemicals (for example, through degradation) or subsequent exposure in a secondary receiving environment, needed to be understood (DoEE 2017b). Initially simple models with conservative estimates were used in the tiered approach. For modelling higher tiers, chemical specific information for the prediction of degradation and mobility from one receiving environment to another was required. The two parameters of most interest were the DT50, used to determine the time taken for 50% of the chemical to degrade in a given environmental compartment, and the soil partitioning coefficient (Kd), which is used to determine the mobility of chemicals from soil to water or water to sediment. In addition, Henry's Law constant allowed the estimation of partitioning between water and air for volatile chemicals.

1.10.1 Parameters

Values for DT50 in soil, sediment and water, and values for Kd are not routinely measured for industrial chemicals (EPHC 2009). Given this, DT50 and Kd values were modelled from semi-quantitative estimates of chemical biodegradability, and from extrapolations of the laboratory measurements routinely made for industrial chemicals.

1.10.2 DT50 value data sources

Data for the determination of DT50 values was identified in the online Persistence Bioaccumulation Toxicity (PBT) profiler (Environmental Health Analysis Center 2012), the OECD QSAR Toolbox v2.2 (OECD 2013a), Catalogic (LMC 2011) and published data from the OECD existing chemicals database. General knowledge on certain surfactants (Madsen et al. 2001) was also considered in the determination of half-lives but insufficient information was found. There were no reliable or known biodegradation values for environmental water, soil or sediment for any of the chemicals associated with coal seam gas operations.

1.10.3 PBT profiler

The PBT profiler (Environmental Health Analysis Center 2012) was accessed online. The PBT profiler is based on the BIOWIN3 program (US EPA 2000-2011), which consists of an expert panel's semi-quantitative estimates of chemical biodegradability and an assumption of pseudo, first-order kinetics (Boethling et al. 1994). The methodology is not based directly on the ease of biotic, oxidative degradation. However, the accuracy of PBT profiler predictions has been evaluated by considering the predictions of a chemical being readily biodegradable or non-readily biodegradable against measured data from a subset of studies which assessed the ease of biotic, oxidative degradation (OECD 301B, 301C, 301D and 302B). Correct predictions were evaluated and it was found that the predicted values correlated well with ease of biotic, oxidative degradation studies (Boethling et al. 2004a and 2004b).

Certain chemicals associated with coal seam gas operations are inorganic compounds, organic salts with unusual counter ions other than Na^+, K^+ and NH_4^+, compounds with molecular weights > 1 000 g/mol and chemicals with unknown or variable composition (UCVB). These chemicals cannot be modelled by the PBT profiler. In addition, surfactant endpoints presented within the PBT profiler were treated with caution (Environmental Health Analysis Centre 2012).

1.10.4 QSAR Toolbox

QSAR Toolbox is software produced by LMC, in cooperation with the OECD and ECHA. It contains a comprehensive database of experimental results from the literature for thousands

of chemicals, as detailed previously (see Section 1.10.1). The output values from QSAR Toolbox are expressed as % degradation in the test timeframe.

1.10.5 Catalogic

Catalogic (LMC 2011) is proprietary software able to model the degradation of chemicals based on mechanistic considerations of degradation including catalysing enzymes, enzyme inhibitors or promoters. The probabilities of the degradation pathways occurring has been built and parameterised on the basis of a set of 583 kinetic curves with more than 15 000 Biological Oxygen Demand (BOD) values which were measured using the ease of biotic, oxidative degradation studies and in particular the OECD 301F test and other OECD TGs (Dimitrov et al. 2011). The output values from Catalogic include the time taken for a chemical to reach half its concentration via mineralisation, biotic degradation in air, and due to degradation from carbon dioxide, water and chemical elements (ultimate half-life).

In addition, Catalogic includes a database that was collated using monographs, internet databases, and articles on the microbial degradation of chemicals (ibid).

1.10.6 Published sources

The following sources of published data were used as sources of data for quality control purposes (Table A.10).

Table A.10 Quality control from published sources

CAS RN	Chemical name	Reference
107-21-1	1,2-Ethanediol	OECD (2009a)
107-22-2	Ethanedial	OECD (2003a)
108-10-1	2-Pentanone, 4-methyl-	OECD (2011b)
111-30-8	Pentanedial	OECD (2001b)
111-76-2	Ethanol, 2-butoxy-	OECD (2007b)
111-90-0	Ethanol, 2-(2-ethoxyethoxy)-	OECD (2007c)
CBI	Ester alcohol	OECD (2002a)
56-81-5	1,2,3-Propanetriol	OECD (2005a)
64-17-5	Ethanol	OECD (2005b)
67-56-1	Methanol	OECD (2007d)
67-63-0	2-Propanol	OECD (2002b)
7727-54-0	Peroxydisulfuric acid, diammonium salt	OECD (2006a)
7757-82-6	Sulfuric acid, disodium salt	OECD (2006b)
7757-83-7	Sulfurous acid, disodium salt	OECD (2009b)
7758-19-2	Chlorous acid, sodium salt	OECD (2009c)
7783-20-2	Sulfuric acid, diammonium salt	OECD (2006c)
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	OECD (2004b)

Suitable data for surfactant analogues were sought (Madsen et al. 2001). However, only data on the ease of biotic, oxidative degradation were available. These require Kow values to be extrapolated to DT50 values in soil and water. As previously described, Kow values cannot be established for surfactants and suitable data for surfactant analogues were therefore not available.

1.10.7 Data sources for Kow

1.10.7.1 Study data

Study data for the Kow for chemicals were sourced from QSAR Toolbox v2.2 (OECD 2013a) and Catalogic (LMC 2011).

1.10.7.2 Modelled data

Where no measured values were available, modelled values were obtained from Catalogic.

1.10.8 Determination of Kd and Koc from Kow

The soil-water partition coefficient (Kd) was determined using a series of accepted conversions from the Kow values determined by the standard studies discussed above (see Section 1.10.1).

The Kd was determined using Equation A.1 (EPHC 2009) where % O.C. (organic carbon) in soil was assumed to be 1% in Australia based on values obtained from ANRA (2001):

$$\mathrm{Kd} = \frac{\mathrm{K_{oc}} \times \%\ \mathrm{O.C.}}{100} \qquad \text{[Equation A.1]}$$

The log Koc of a chemical is well-correlated with the log Kow and was determined according to Equation A.2 (US EPA 1996):

$$\log \mathrm{K_{oc}} = 0.983 \times \log \mathrm{K}_{ow} + 0.00028 \qquad \text{[Equation A.2]}$$

The Koc values were then determined from the log Kow.

1.10.9 Henry's Law constant

Two sources of data were identified for obtaining Henry's Law constant. These were QSAR Toolbox v2.2 (OECD 2013a) and the published data identified in Table A.9 and Table A.10. The values were presented in units of atm.m^3/mol and converted to Pa.m^3/mol using the standard conversion factor of 1.013 × 10^5 Pa/atm (Aylward and Findlay 1974).

1.11 Data selection

1.11.1 Determination of DT50 endpoints: criteria

Of the five data sources, only the PBT profiler directly estimated DT50 values for soil, water and sediment. The published data in Table A.10 was used to categorise the chemicals' ease of biotic, oxidative degradation according to the four categories (readily biodegradable, readily biodegradable failing 10-day window, inherently biodegradable and non-biodegradable). These data could then be extrapolated to DT50 values in soil and water using the methodology of EC (2003) cited in DoEE (2017c) (see Table A.11).

Data from QSAR Toolbox and Catalogic had the additional complexity that it had to be further extrapolated from percentage degradation or ultimate half-life to one of the four categories of ease of biotic, oxidative degradation.

Table A.11 Estimation soil half-life from results of biodegradability studies and Kd

Kd_{soil} (L/kg)	**Readily biodegradable**	**Readily biodegradable failing 10 day window**	**Inherently biodegradable**
Kd_{soil} (L/kg)	Soil half-lives days	Soil half-life days	Soil half-life days
≤ 100	30	90	300
> 100 to ≤ 1 000	300	900	3 000
> 1 000 to ≤ 10 000	3 000	9 000	30 000
Not applicable	Water half-life days	Water half-life days	Water half-life days
Not applicable	15	50	150

For chemicals that were determined to be non-biodegradable, a default value of 100 000 days was used for soil and water regardless of the Kd value for soil (EPHC 2009).

As the choice of data critically affects the validity of environmental models (DoEE 2017b and 2017c), a hierarchy of data quality was determined based on the extent of extrapolation. The hierarchy was as follows:

- Initially only data from the PBT profiler and published data was considered as no extrapolation was required.
- If these data differed by less than one order of magnitude, then the PBT profiler value took precedence as this method took into better account chemical degradation pathways.
- Chemicals with no data from the PBT profiler had their half-lives calculated from the published categories of ease of biotic, oxidative degradation in accordance with EC (2003).
- If the PBT profiler and published data differed by more than one order of magnitude, consideration was given to the catabolic pathways described by Catalogic and % degradation reported by Catalogic and QSAR Toolbox.

1.11.2 Determination of DT50 endpoints: findings

It was found that the half-lives from both the PBT profiler and QSAR Toolbox sources were generally in good agreement (less than one order of magnitude), with the only exception being ethanol, 2,2',2''-nitrilotris- (102-71-6). The PBT profiler indicated a soil half-life of 30 days while experimental data for the ease of biotic, aerobic degradation found that it did not degrade (OECD 2001a) and had an approximate half-life of 100 000 days. To resolve this conflict in predictions of half-life, further analysis was performed by Catalogic using the BOD 28 days MITI (OECD 301C) v3.04 simulator to examine the degradation pathways. In addition, % degradation from QSAR Toolbox and Catalogic was examined.

It was found that Catalogic concurred with the published data (OECD 2001a) in that there was no known degradation pathway for ethanol, 2,2',2''-nitrilotris- (Table A.11). Additionally, QSAR Toolbox recorded zero per cent degradation in 14 days and Catalogic ascribed the

ultimate half-life as > 10 years. Accordingly, the assigned value of 100 000 days took precedence over the 30 days modelled by the PBT profiler.

1.11.3 Determination of Koc endpoints: criteria

The Koc values were derived from three sources (QSAR Toolbox, Catalogic and published data in Table A.10). Where the values were indicated to be measured, including those in the training set for Catalogic and where they were within one order of magnitude, the average (arithmetic) of all the values was taken.

1.11.4 Determination of Koc: findings

Most of the Koc values were in good agreement. The only exception was ethanaminium, 2-hydroxy-N,N,N-trimethyl-, chloride (67-48-1). Catalogic modelled a Koc value of 8.56×10^{-6}, while OECD (2005c) reported a value of 2.34. Since the value from OECD (2005c) has been peer-reviewed from a study, it took precedence over the modelled value.

1.11.5 Determination of Henry's Law constant: criteria

Where data between the various sources differed by less than 10%, the mean (arithmetic) was taken. Professional judgement was used for differences in values exceeding 10%.

1.11.6 Determination of Henry's Law constant: findings

More than one source of data was found for Henry's Law constants for ethanol (64-17-5), methanol (67-56-1) and 2-propanol (67-63-0). The values for methanol and 2-propanol varied by less than 10% and the average values were taken. Indeed the variation for methanol appeared to be from rounding with less than 0.1% difference. According to OECD (2005b), ethanol has a Henry's Law constant of 0.61 $Pa.m^3/mol$ – this differs more than 10% from the value of 0.51 $Pa.m^3/mol$ obtained from QSAR Toolbox. However, the test reported by OECD (2005b) was conducted at 15°C rather than the more standard 20 or 25°C. Accordingly, the value for ethanol chosen was 0.61 $Pa.m^3/mol$.

1.11.7 Conversions from soil to water and sediment

The PBT profiler (Environmental Health Analysis Center 2012) recommends the following conversions of half-lives in water, soil and sediment (Table A.12). The conversions have been based on differences in microbial activity and aerobic conditions.

Table A.12 DT50 conversion factors for environmental compartments

Conversion multiply DT50 by	Water	Soil	Sediment
Water	1	0.5	0.11
Soil	2	1	0.22
Sediment	9	4.5	1

The final values found for each chemical are provided in Table A.13 and Table A.14.

Table A.13 Physico-chemical properties for drilling chemicals

CAS RN	Chemical name	Soil-Water partition coefficient KOC	Soil-Water partition coefficient log Kow	Distribution coefficient Kd (KOC x foc*)	Water solubility (mg/L)	Henry's Law constant Hcc (Pa-m^3/mol)	DT50$_{soil}$ (days)
CBI	2-Ethylhexanol heavies	485	2.640	-	1285	2.68	17
107-22-2	Ethanedial	0.0236	-1.599	2.36E-04	1000000	3.37E-04	30
111-30-8	Pentanedial/ Glutaraldehyde	0.663	0.806	8.20E-03	710000	-	30
11138662	Xanthan gum	-	-	-	-	-	-
1305620	Calcium hydroxide ($Ca(OH)_2$)	-	-	-	1650 (20°C)	-	-
1310732	Sodium hydroxide (NaOH)	-	-	-	-	-	-
144-55-8	Carbonic acid, monosodium salt	1.14E-04	-3.875	1.143E-06	1000000	-	-
CBI	Ester alcohol	-	-	-	-	-	30
497198	Carbonic acid, disodium salt	-	-	-	-	-	-
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)						
64-17-5	Ethanol	0.727	-0.136	7.41E-3	452000	0.507	17
64742-47-8	Distillates, petroleum, hydrotreated light	1.35E6	6.025	13 500	0	-	-
67-56-1	Methanol	0.239	-0.610	2.01E-03	1000000	0.461	17
67-63-0	2-Propanol	1.87	0.268	0.0135	2.87E5	0.821	30
CBI	Organic sulfate	-	-	-	-	-	-
CBI	Organic acid salt	1870	3.216	18.7	0	-	-
7447407	Potassium chloride (KCl)	-		-	-	-	-
7757837	Sulfurous acid, disodium salt	-	-	-	-	-	-
7758169	Diphosphoric acid, disodium salt	-	-	-	-	-	-
7778805	Sulfuric acid, dipotassium salt	-	-	-	12000 (25°C)	-	-
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	0.023	-1.616	2.25E-04	1000000	4.39E-09	90
CBI	Polymer with substituted alkylacrylamide salt		-0.78	2.20E-03	956000	0.0002	-
9000-30-0	Guar gum	7.08E-07	-6.15	7.08E-09	1000000	-	-
CBI	Polymer	8.32E+16	16.92	8.32E+14	0.0000010	-	-

Note. Physico-chemical values were estimated using Catalogic (KOWWINTM) with various levels of reliability.

Table A.14 Physico-chemical properties for hydraulic fracturing chemicals

CAS RN	Chemical name	Soil-Water partition coefficient KOC	Soil-Water partition coefficient log Kow	Distribution coefficient Kd (KOC x foc*)	Water solubility (mg/L)	Henry's Law constant K_H (Pa-m^3/mol)	$DT50_{soil}$ (days)
10043-35-3	Boric acid (H_3BO_3)	0.607	-0.213	6.07E-03	1000000	-	-
10043524	Calcium chloride ($CaCl_2$)	-	-	-	-	-	-
107-21-1	1,2-Ethanediol	0.059	-1.16	5.95E-04	1000000	6.08E-03	17
108-10-1	2-Pentanone, 4-methyl-	17.597	1.13	0.176	19000	14.0	30
111-76-2	Ethanol, 2-butoxy-	5.425	0.548	0.0543	155000	0.162	17
111-90-0	Ethanol, 2-(2-ethoxyethoxy)-	0.252	-0.666	2.52E-03	1000000	2.26E-03	30
1310732	Sodium hydroxide (NaOH)	-	-	-	-	-	-
141-43-5	Ethanol, 2-amino-	0.043	-1.56	4.31E-04	1000000	-	30
144-55-8	Carbonic acid, monosodium salt	1.14E-04	-3.87	1.14E-06	1000000	-	-
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	0.464	-0.328	4.64E-03	323000	-	-
2634-33-5	1,2-Benzisothiazol-3(2H)-one	4.229	0.616	0.0423	22200	-	30
2682-20-4	3-Isothiazolone, 2-methyl-	0.152	-0.804	1.52E-03	959000	-	30
497-19-8	Carbonic acid, disodium salt	-	-	-		-	-
52-51-7	1,3-Propanediol, 2-bromo-2-nitro-	0.235	-0.619	2.35E-03	1000000	1.35E-06	30
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	-	-	-	-		-
56-81-5	1,2,3-Propanetriol	0.021	-1.60	2.12E-04	1000000	1.75E-03	30
CBI	Amine salt		-4.57		18200	-	30
CBI	Inner salt of alkyl amines (Talc)	4.738	0.664	0.0474	2.38	-	-
CBI	Ethoxylated fatty acid (1)	8.20E-03	-2.05	8.20E-05	2240	-	-
CBI	Ethoxylated fatty acid (2)	2.78E+16	16.2	2.78E+14	1.00E-06	-	-
CBI	Ethoxylated fatty acid (3)	1440	3.11	14.4	122	-	-
6381-77-7	D-Erythro-hex-2-enonic acid, .gamma.-lactone, monosodium salt	0	-6.81	0	1000000	-	17
6410-41-9	2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-	0	-12.7	0	1000000	-	360
64-17-5	Ethanol	0.741	7.39	7.41E-03	1.87E-04	0.507	17
64-19-7	Acetic acid	0.681	-0.136	6.81E-03	452000	0.0101	17
67-56-1	Methanol	0.201	0.0844	2.01E-03	771000	0.461	17
67-63-0	2-Propanol	1.35	-0.610	0.0135	1000000	0.821	30
68187177	Sulfuric acid, mono-C_{6-10}-alkyl esters, ammonium salts	-	-	-	-	-	-
68439-45-2	Alcohols, C_{6-12}, ethoxylated	25.7	0.268	0.257	287000	-	-
68647-72-3	Terpenes and terpenoids, orange oil	55700	4.67	557	44.4	-	-

CAS RN	Chemical name	Soil-Water partition coefficient KOC	Soil-Water partition coefficient log Kow	Distribution coefficient Kd (KOC x foc*)	Water solubility (mg/L)	Henry's Law constant K_H (Pa-m^3/mol)	$DT50_{soil}$ (days)
7447407	Potassium chloride (KCl)	-	-	-	-	-	-
CBI	Quaternary amine	1.437	-0.616	0.0144	1000000	10.5	-
75-57-0	Methanaminium, N,N,N-trimethyl-, chloride	7.76E-05	-4.04	7.76E-07	6830	-	-
7647010	Hydrochloric acid	-	-	-	-	-	-
7647145	Sodium chloride (NaCl)	-	-	-	-	-	-
7681529	Hypochlorous acid, sodium salt	-	-	-	-	-	-
7727540	Peroxydisulfuric acid ($(HO)S(O)_2)_2O_2$), diammonium salt	-	-	-	-	-	-
7757826	Sulfuric acid, disodium salt	-	-	-	-	-	-
7757837	Sulfurous acid, disodium salt	-	-	-	-	-	-
7758192	Chlorous acid, sodium salt	-	-	-	390	-	-
7775271	Peroxydisulfuric acid ($(HO)S(O)_2)_2O_2$), disodium salt	-	-	-	5.49E+03	-	-
7783202	Sulfuric acid, diammonium salt	-	-	-	764 (20°C)	-	-
7786303	Magnesium chloride ($MgCl_2$)	-	-	-	-	-	-
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	0.023	-1.62	2.25E-4	1000000	4.39E-9	90
81741-28-8	Phosphonium, tributyltetradecyl-, chloride	2.36E6	6.26	23600	0	-	-
9000-30-0	Guar gum	7.08E-07	-6.05	7.08 E-9	1000000	-	-
26062-79-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer	0.004	-2.41	3.57E-05	113	-	-

Note. The physico-chemical value were estimated using Catalogic (KOWWINTM) with various level of reliability.

1.12 References

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Appendix B – Tiering methodology for estimating predicted environmental concentrations

1 Tiering methodology for estimating predicted environmental concentrations

1.1 Introduction

The methodology, equations, parameters and values used to estimate the predicted environmental concentrations (PECs) of each chemical at each point of potential release in aquatic and / or terrestrial environmental receptors are presented in Table B.1 and summarised below. The mathematical equations are based on previous work undertaken by the Department of the Environment as part of the National Coal Seam Gas Chemicals Assessment and reported in the Environmental Exposure Conceptualisation report (DoEE 2017).

The results of the environmental risk assessment obtained by using this methodology are presented as Appendix A.

The exposure scenarios of the risk assessment involved a chemical entering a surface aquatic environment at eight different potential points of release within a coal seam gas working site (Figure B.1). They include:

- an accidental surface spill (of a drilling or hydraulic fracturing chemical) during:
  - transport – a one-off spill during a chemical's transport (by road) between the supplier's warehouse and a regional intermediate storage facility (point of release 1a, Tier 1 only), and between the intermediate storage facility and a well site (point of release 1b). At each point of release, two sub-scenarios are assessed – the chemical entering a waterbody directly, and the chemical entering a waterbody indirectly (via runoff from a nearby spill)
  - storage of chemicals – spills at an intermediate storage facility (point of release 2), and at a well site chemical storage area (point of release 3). At each point of release, the chemical enters a waterbody indirectly (via runoff from a nearby spill), and two sub-scenarios are assessed – a one-off spill, and multiple spills over a period of time
  - use – spills during the use (injection) of chemicals at the well site (point of release 4), and when handling/managing coal seam gas wastewater at the well site (point of release 5). The chemical enters a waterbody indirectly (via runoff from a nearby source), and two sub-scenarios are assessed – a one-off spill, and multiple spills over a period of time

  - storage of waste – spills during the storage of flowback and / or produced water at a wastewater storage area (e.g. dam) in the coal seam gas working site (point of release 6). The chemical enters a waterbody indirectly (via runoff from a nearby source), and two sub-scenarios are assessed – a one-off spill, and multiple spills over a period of time.

- an intentional surface release of a chemical (hydraulic fracturing chemical only) during:
  - dust suppression – the reuse of wastewater for dust suppression within the coal seam gas working site (point of release 7). The chemical enters a waterbody indirectly (via runoff from a nearby source) in a one-off release event
  - irrigation – the reuse of wastewater for irrigation outside of the coal seam gas working site (point of release 8). The chemical enters a waterbody indirectly (via runoff from a nearby source) in a one-off release event.

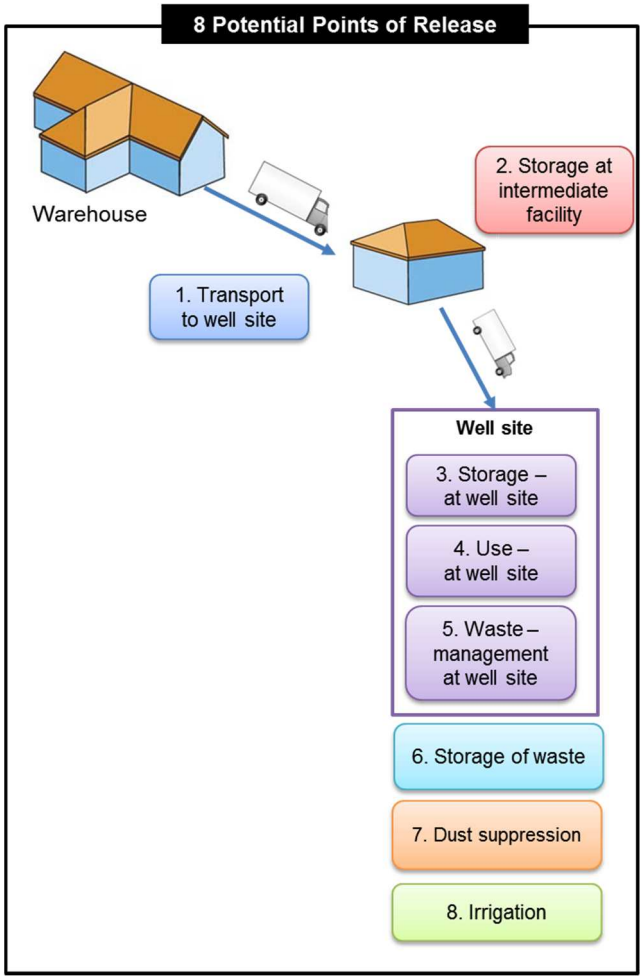

Figure B.1 The eight conceptualised potential points of release from the chemical life-cycle within a coal seam gas working site

Where a point of release is not relevant to a particular coal seam gas working site being assessed, or data are not available, the point of release is not included in the assessment.

1.2 Calculating chemical quantity (*Q*) at points of release

1.2.1 Transport and storage

The chemical quantity that is released from a transport or storage-related spill is calculated by using Release Equation 1 and Input Equation 1, which considers the volume (*V*) and concentration of the chemical (C_f) being transported (*T*) or stored (*S*), and the fraction of the load spilling (i) in a transport, storage or use incident.

1.2.2 Use at the well site

The chemical quantity that is released (spilled) during use at the well site is calculated by using Release Equation 3 and Input Equation 1 (DoEE 2017), which considers the volume (V_U) and concentration (C_D) of the final diluted process fluid injected into the well during a drilling or hydraulic fracturing operation, and the fraction of the load spilling (i_S) in a use-related incident.

1.2.3 Waste management / handling (at the well site, immediately after operations)

The chemical quantity that is released from the management / handling of waste from a single well (Q_{xUS}) is calculated by using Release Equation 4 and Input Equation 1 (DoEE 2017), which considers the volume (V_U) and concentration ranges (C_D) of the final diluted process fluid injected into the well during a drilling or hydraulic fracturing operation, the portion of chemical returned from the well (i_{UR}), and the portion of chemical spilled subsequent to injection (i_{US}).

1.2.4 Waste disposal (main storage dam)

The chemical quantity that is released in waste fluids from a storage dam (i.e. flowback and / or produced waters containing hydraulic fracturing chemicals) is calculated by using Release Equations 6 to 9. These equations consider the volume (V_U) and concentration ranges (C_D) of the final diluted process fluid injected into the well during a hydraulic fracturing operation, the portion of hydraulic fracturing chemical returned from the well (i_{UR}), the quantity of geogenic chemicals in the flowback and / or produced water released from a well (Q_{GEO}), and the contaminant in flowback and / or produced water released from various wells ($Q_{xWCP_i}$and n).

1.3 Calculating predicted environmental concentrations (PEC)

The calculation of PECs is undertaken initially for direct spills and subsequently for indirect spills, where a range of factors are used to account for volatilisation and partitioning into the air, sediment and vegetation. Calculations for terrestrial receptors are required to estimate indirect aquatic PECs.

1.3.1 Aquatic receptors

The chemical concentration in the receiving aquatic environment (without volatilisation and sedimentation) is calculated by Exposure Equation 1 (DoEE 2017):

$$PEC_{aquatic} = \frac{Q_{xReleasePoints}}{V_{water}} \times 10^6 \ mg/L \qquad \text{[Equation B.1]}$$

The volume of the aquatic receptor is calculated by using Exposure Equation 3 (DoEE 2017):

$$V_{water} = V_{environmental} + V_{contaminated} + V_{uncontaminated}$$ [Equation B.2]

The aquatic PEC after volatilisation and sedimentation is calculated as follows:

$$PEC_{aquatic} = PEC_{initial\ aquatic} - (PEC_{air} + PEC_{sediment})$$ [Equation B.3]

Volatilisation from the aquatic receptor is calculated from Exposure Equation 19 and Exposure Equation 20 (DoEE 2017):

$$K_{air-\!-\!-water} = H/R \times T$$ [Equation B.4]

$$PEC_{air} = K_{air-water} \times PEC_{water}$$ [Equation B.5]

Sedimentation from the water column in the aquatic receptor is calculated from Exposure Equation 21 and Exposure Equation 22 (DoEE 2017):

$$K_{sediment_water} = 0.8 + (0.2 \times {}^{K_d}/_{1000}) \times \rho_{solid}$$ [Equation B.5]

$$PEC_{sediment} = \frac{K_{sediment_water}}{\rho_{sediment}} \times 1000 \times PEC_{initialaquatic}$$ [Equation B.6]

1.3.2 Terrestrial receptors

1.3.2.1 Direct release – terrestrial receptor

The chemical quantity that is released from storage or use spill is calculated by using Release Equation 1 and Input Equation 1 (DoEE 2017).

The chemical concentration in the receiving terrestrial environment is calculated by using Exposure Equation 4 (DoEE 2017):

$$PEC_{soil} = \frac{Q}{A \times d \times \rho} \times 10^6\ mg/kg$$ [Equation B.7]

Exposure Equation 4 (DoEE 2017) is dependent on the spread of the spill. This requires additional equations in relation to the height and area of the spill. The height of the spill is calculated by using Exposure Equation 5 (DoEE 2017) and the area is calculated by Exposure Equation 6 (DoEE 2017):

$$h = \sqrt{\frac{1-cos(\beta)\times\sigma}{\rho\times g}}$$ [Equation B.8]

$$A = \frac{V}{h}$$ [Equation B.9]

1.3.3 Runoff

1.3.3.1 Indirect release – aquatic receptor

The chemical quantity (*Q*) that is released from storage or use spills is calculated by Release Equation 1 and Input Equation 1 (DoEE 2017).

An indirect release occurs when the chemical quantity is initially released to the terrestrial environment with a fraction then transported overland with runoff water ultimately to an aquatic receptor. The quantity of chemical in the runoff water is calculated by Exposure Equation 9 (DoEE 2017c). This equation relates the quantity of chemical with the ratio of the amount of runoff and the total water input (i.e. precipitation) and other variables relating to factors such as slope and foliar interception.

$$L\%_{runoff} = \left(\frac{R}{\Psi}\right) \times Cr_{soil_{surface}} \times f1slope \times f2bufferzone \times f3foliar_{application} \times heterogeneity_{factor} \times 100 + suspended_{contaminants}\%$$ [Equation B.10]

The value for $Cr_{soil_surface}$ is calculated from the chemical half-life (DT50) and K_d values as described by Exposure Equation 10 (DoEE 2017), where K_d is derived from Exposure Equation 15 (DoEE 2017):

$$C_{rsoil_surface} = e^{(-3\,ln\,2/DT50soil)} \times [1/(1+K_d)]$$ [Equation B.11]

$$K_d = K_{oc} \times OC\%/100$$ [Equation B.12]

Other variables, such as f1slope, f2buffer_zone, f3foliar_application, and runoff (R), are calculated by Exposure Equations 11, 12, 13, and 14 respectively (DoEE 2017):

$$\text{f1slope} = 0.02153 \times \text{slope} + 0.001423 \times \text{slope}^2 \text{ for slope} < 20\%$$
$$= 1 \text{ for slope} \geq 20\%$$ [Equation B.13]

$$f2buffer_\text{zone} = 0.83^{buffer\,width}$$ [Equation B.14]

$$f3foliar_application = 1 - F_{int} \times 0.5$$ [Equation B.15]

$$R = (\Psi - 0.2S)^2/(\Psi + 0.8S)$$ [Equation B.16]

The variable *S* in Exposure Equation 14 (DoEE 2017) is the potential maximum retention after runoff begins and is dependent on curve number (CN) as described by the following equation:

$$S = 1000/CN - 10 \quad \text{[Equation B.17]}$$

The chemical quantity in the runoff water at the edge of the field is calculated as a fraction of the quantity of chemical released and is designated Q_R. This variable has not been defined in the Environmental Exposure Conceptualisation report (DoEE 2017) but has been recorded here to distinguish it from the release quantity. The fraction of the quantity of chemical released is represented by the following equation:

$$\mathrm{Q_R} = \mathrm{Q_{ReleasePoints}} \times L\%_{run-off} \quad \text{[Equation B.18]}$$

1.3.4 Single releases

A single release is represented by one working site with eight potential release points each releasing one time to an aquatic receptor.

1.3.5 Multiple releases

The multiple release scenario is represented by one working site with eight potential release points each releasing a number of times to an aquatic receptor. The number of releases represents the number of wells in the working site.

The values used in the different modelling parameters are described in the tables below.

Table B.1 Equations, parameters and values used to estimate the PECs of drilling and hydraulic fracturing chemicals spilled or intentionally released as part of a coal seam gas extraction operation

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
POINTS OF RELEASE					
Calculating the quantity of chemical likely to be spilled or intentionally released under different release scenario (i.e. points of release).			Tier 1 values use bounding estimate values [4]. The values for the generic assessment are based on the mean of all the new bounding estimate values provided by industry. The values from the NICNAS survey (Appendix A) are used for those chemicals without new data from industry.	Tier 2 use high-end estimate values [5]. The bioregional values are based on the mean of all the new high-end estimate values provided by industry for each specific bioregion.	Tier 3 values should always represent the central tendency values [6]. The site specific values are based on central tendency values provided by each working site in the new industry data.
Transport from warehouse to intermediate storage					
$= Q_T \times i_T$	$\boldsymbol{Q_{xT}}$	**Quantity of chemical spilled during transport (mg)**	**Release equation 1**	**Release equation 1**	**Release equation 1**
	Q_T	Quantity of drilling or hydraulic fracturing chemical transported (mg)	As calculated by Input equation 1	As calculated by Input equation 1	As calculated by Input equation 1
	i_T	Fraction of a truck load spilling in an accident	Liquid = 1.0 Solid = 0.5 (100%)	Liquid = 0.9 Solid = 0.45 (90%)	Liquid = 0.5 Solid = 0.25 (50%)
$Q_T = V_T \times C_f$	$\boldsymbol{Q_T}$	**Quantity of chemical transported (mg)**	**Input equation 1**	**Input equation 1**	**Input equation 1**
	V_T	Volume of drilling and hydraulic fracturing formulations transported (L or kg)	The values used for V_T and C_f are provided in Table B.2 to Table B.35.		
	C_f	Concentration of chemical in formulation (mg/kg or mg/L)			
Transport from intermediate storage to well site storage area					
$Q_{xT} = Q_T \times i_T$	$\boldsymbol{Q_{xT}}$	**Quantity of chemical spilled during transport (mg)**	**Release equation 1**	**Release equation 1**	**Release equation 1**
	Q_T	Quantity of drilling or hydraulic fracturing chemical transported (mg)	As calculated by Input equation 1	As calculated by Input equation 1	As calculated by Input equation 1
	i_T	Fraction of a truck load spilling in an accident	Liquid = 1.0 Solid = 0.5 (100%) [7]	Liquid = 0.9 Solid = 0.45 (90%) [8]	Liquid = 0.5 Solid = 0.25 (50%) [9]

[4] Highest possible exposure.
[5] Reasonable maximum volume of release, maximum concentration and maximum exposure.
[6] Represent the average or typical individual in a population, usually near the median or 50th percentile of the population distribution.
[7] Highest possible exposure.
[8] Reasonable maximum, reasonable worst-case, and maximum exposure.
[9] Represent the average or typical individual in a population, usually near the median or 50th percentile of the population distribution.

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
$= V_T \times C_f$	$\boldsymbol{Q_T}$	**Quantity of chemical transported (mg)**	**Input equation 1**	**Input equation 1**	**Input equation 1**
	V_T	Volume of drilling and hydraulic fracturing formulations transported (L or kg)	The values used for $V_T$and $C_f$are provided in Table B.2 to Table B.35.		
	C_f	Concentration of chemical in formulation (mg/kg or mg/L)			
Intermediate storage facility					
$Q_{xS} = Q_S \times i_S$	$\boldsymbol{Q_{xS}}$	**Quantity of chemical spilled at intermediate storage locations prior to operations (mg)**	**Release equation 3**	**Release equation 3**	**Release equation 3**
	Q_S	Quantity of drilling or hydraulic fracturing chemical quantities stored at intermediate locations prior to operations (mg)	As calculated by Input equation 1	As calculated by Input equation 1	As calculated by Input equation 1
	i_S	Fraction of a stored load spilling in an incident	Liquid = 1.0 Solid = 0.5 (100%)	Liquid = 0.9 Solid = 0.45 (90%)	Liquid = 0.5 Solid = 0.25 (50%)
$Q_S = V_s \times C_f$	$\boldsymbol{Q_S}$	**Quantity of chemical stored at intermediate storage locations prior to operations (mg)**	**Input equation 1**	**Input equation 1**	**Input equation 1**
	Vs	Volume of drilling and hydraulic fracturing formulations stored (kg or L)	The values used for $V_T$and $C_f$are provided in Table B.2 to Table B.35.		
	C_f	Concentration of a specific chemical in a drilling or hydraulic fracturing fluid system (mg/kg or mg/L)			
Well site storage facility					
$Q_{xS} = Q_S \times i_S$	$\boldsymbol{Q_{xS}}$	**Quantity of chemical spilled from well site storage (mg)**	**Release equation 3**	**Release equation 3**	**Release equation 3**
	Q_S	Quantity of drilling or hydraulic fracturing chemical stored at well site operation (mg)	As calculated by Input equation 1	As calculated by Input equation 1	As calculated by Input equation 1
	i_S	Fraction of a stored load spilling in an incident	Liquid = 1.0 Solid = 0.5 (100%)	Liquid = 0.9 Solid = 0.45 (90%)	Liquid = 0.5 Solid = 0.25 (50%)
$Q_S = V_s \times C_f$	$\boldsymbol{Q_S}$	**Quantity of chemical stored at well site operation (mg)**	**Input equation 1**	**Input equation 1**	**Input equation 1**
	Vs	Volume of drilling or hydraulic fracturing fluid systems stored on well site (L or kg)	The values used for $V_S$and $C_f$are provided in Table B.2 to Table B.35.		

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
	C_f	Concentration of a specific chemical in a drilling or hydraulic fracturing fluid system (mg/kg or mg/L)			
Use at the well site					
$Q_{xUP} = Q_U \times i_S$	$\boldsymbol{Q_{xUP}}$	**Quantity of chemical spilled during use at the well site (mg)**	**Release equation 3**	**Release equation 3**	**Release equation 3**
	Q_U	Quantity of drilling or hydraulic fracturing chemical to be used at a single well site (mg)	As calculated by Input equation 1A	As calculated by Input equation 1A	As calculated by Input equation 1A
	i_S	Fraction of a load spilling in an accident	Liquid = 1.0 Solid = 0.5 (100%)	Liquid = 0.9 Solid = 0.45 (90%)	Liquid = 0.5 Solid = 0.25 (50%)
$Q_U = C_D \times V_U$	$\boldsymbol{Q_U}$	**Quantity of chemical to be used at a single well site (mg)**	**Input equation 1A**	**Input equation 1A**	**Input equation 1A**
	V_U	Total volume of the final diluted process fluid injected into the well during drilling or hydraulic fracturing operations (kg or L)	The values used for V_U and C_D are provided in Table B.2 to Table B.35.		
	C_D	Chemical concentration ranges in the final diluted process fluid injected into the well during drilling or hydraulic fracturing operations (mg/kg or mg/L)			
Waste management and storage (at the well site)					
					As there were no specific data on flowback and / or produced water chemical composition and concentration, 100% recovery of the injected drilling and hydraulic fracturing chemical was assumed for the Tier 1 assessment. There was also no information available on geogenic contaminants. The site storage volumes provided by industry were considered.
$Q_{xUS} = [Q_U \times i_{UR} \times i_{US}]$	$\boldsymbol{Q_{xUS}}$	**Quantity of chemical in wastewater[10] spilled subsequent to operations (mg)**	**Release equation 4**	**Release equation 4**	**Release equation 4**
	Q_U	Quantity of drilling or hydraulic fracturing chemical in injection fluid (mg)	As calculated by Input equation 1A	As calculated by Input equation 1A	As calculated by Input equation 1A
	i_{UR}	Portion of drilling or hydraulic fracturing chemical returned from the well	1.0	0.90	0.50
	i_{US}	Portion of chemical (unintentionally) released subsequent to injection	1.0	0.90	0.50

[10] Flowback and / or produced waters.

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
– $Q_U = C_D \times V_U$	**Q_U**	**Quantity of chemical in wastewater at a single well site (mg)**	**Input equation 1A**	**Input equation 1A**	**Input equation 1A**
	– V_U	Total volume of the final diluted process fluid injected into the well during drilling or hydraulic fracturing operations (kg or L)	The values used for V_U and C_D are provided in Table B.2 to Table B.35.		
	– C_D	Chemical concentration ranges in the final diluted process fluid injected into the well during drilling or hydraulic fracturing operations (mg/kg or mg/L)			
Waste disposal (main dam storage)					
			Hydraulic fracturing chemicals only		
$Q_{xWD} = Q_{xWtot} \times (i_{AM} \times i_{AMR} + i_{UAM})$	**Q_{xWD}**	**Total contaminant released from waste disposal activities**	**Release equation 9**	**Release equation 9**	**Release equation 9**
	Q_{xWtot}	Total quantity of contaminant in stored wastewater (mg)	As calculated by Release equation 8	As calculated by Release equation 8	As calculated by Release equation 8
	i_{AM}	Portion of wastewater treated/amended and released	0	0	0
	i_{AMR}	Portion of contaminants released after treatment	0	0	0
	i_{UAM}	Portion of wastewater not treated (unamended)	1	**1**	**1**
– $Q_{xWtot} = \sum_i^n Q_{xWCP_i}$	**Q_{xWtot}**	**Total quantity of contaminant in stored wastewater (mg)**	**Release equation 8**	**Release equation 8**	**Release equation 8**
	– Q_{xWCP_i}	Quantity of contaminant in the flowback or produced water released from each well (mg)	As calculated by Release equation 6 and Release equation 7	As calculated by Release equation 6 and Release equation 7	As calculated by Release equation 6 and Release equation 7
	– n	Number of wells that feed into the main dam storage			
$Q_{xWCP} = [Q_U \times i_{UR}]$	**Q_{xWCP}**	**Contaminant quantity in wastewater from a well (mg)**	**Release equation 6**	**Release equation 6**	**Release equation 6**
	Q_U	Quantity of hydraulic fracturing chemical in injection fluid (mg)	As calculated by Input equation 1A	As calculated by Input equation 1A	As calculated by Input equation 1A
	i_{UR}	Portion of hydraulic fracturing chemical returned from the well	1.0	0.90	0.50
– $Q_U = C_D \times V_U$	**Q_U**	**Quantity of chemical in injection fluid (mg)**	**Input equation 1A**	**Input equation 1A**	**Input equation 1A**
	– V_U	Total volume of the final diluted process fluid injected into the well	The values used for V_U and C_D are provided in Table B.2 to		

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
		during hydraulic fracturing operations (kg or L)	Table B.35.		
	– C_D	Chemical concentration ranges in the final diluted process fluid injected into the well during hydraulic fracturing operations (mg/kg or mg/L)			
$Q_{xWCP} = Q_{GEO}$	**Q_{xWCP}**	**In the case of geogenics, contaminant quantity in wastewater (mg)**	**Release equation 7**	**Release equation 7**	**Release equation 7**
	Q_{GEO}	Quantity of geogenic chemicals in the flowback and / or produced water released from a well (mg)	As calculated by Release equation 7A	As calculated by Release equation 7A	As calculated by Release equation 7A
$Q_{GEO} = C_{GEO} \times V_U$	**Q_{GEO}**	**Quantity of geogenic chemicals in the flowback and / or produced water released from a well (mg)**	**Release equation 7A**	**Release equation 7A**	**Release equation 7A**
	C_{GEO}	Concentration of geogenic chemicals in waste fluids (mg/L)	Nil (no data)	Nil (no data)	Nil (no data)
	– V_U	Volume of flowback and / or produced water released from a well (L)	The values used for V_U are provided in Table B.2 to Table B.35.		
Irrigation and dust suppression					
			Hydraulic fracturing chemicals only		
	$C_{irrigation}$	**Concentration of a chemical in wastewater used for irrigation or dust suppression (mg/L)**	**Release equation 10A**	**Release equation 10A**	**Release equation 10A**
$C_{irrigation} = Q_{xWD}/V_s$	Q_{xWD}	Quantity of chemical in multi-well wastewater dam (mg)	As calculated by Release equation 9 (see previous, under 'Waste disposal (main dam storage)'	As calculated by Release equation 9 (see previous, under 'Waste disposal (main dam storage)'	As calculated by Release equation 9 (see previous, under 'Waste disposal (main dam storage)'
	V_s	The total volume waste fluid used for irrigation/dust suppression (L) (Volume of multi-well waste water dam)	840 ML[11]	Calculated from industry data (based on injected volumes and number of wells in the working site) and assumed losses	Calculated from industry data (based on injected volumes and number of wells in the working site) and assumed losses
$PEC_{edgeoffield} = Q_{irrigationOrDustS}/V_{contaminated}$	**PEC*edgeoffield***	**Contaminant concentration at the edge of field**	**Release equation 13**	**Release equation 13**	**Release equation 13**
	$Q_{irrigationOrDustS}$	Quantity of chemical applied to area via irrigation (mg/L)	Calculated as per release equation 14 (for 1 ha)	Calculated as per release equation 14 (for 1 ha)	Calculated as per release equation 14 (for 1 ha)
	V*contaminated*	Volume of contaminated water running off from area (equivalent to rainfall volume across given area) (L)	Calculated as per release equation 14 (for 1 ha)	Calculated as per release equation 14 (for 1 ha)	Calculated as per release equation 14 (for 1 ha)

[11] Maximum dam capacity (Coffey Environments 2012).

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
$Q_{irrigationOrDustS} = L\%runoff \times W$	$\boldsymbol{Q_{irrigationOrDustS}}$	**Quantity of chemical applied to area via irrigation or dust suppression**	**Release equation 14**	**Release equation 14**	**Release equation 14**
	W	Chemical application rate (g/ha/y)	As calculated by Release equation 12	As calculated by Release equation 12	As calculated by Release equation 12
	$L\%runoff$	Fraction of chemical in runoff water	As calculated by Exposure equation 9 (see below under 'Runoff')	As calculated by Exposure equation 9 (see below under 'Runoff')	As calculated by Exposure equation 9 (see below under 'Runoff')
$W = A \times C_{irrigation}$	$\boldsymbol{W}$	**Chemical application rate (g/m^2)**	**Release equation 12**	**Release equation 12**	**Release equation 12**
	A	Application rate of wastewater containing hydraulic fracturing chemicals for irrigation (L/m^2)	1000/y	1000/y	100/irrigation event
	$C_{irrigation}$	Concentration of a chemical in wastewater dam (g/L)	As calculated by Release equation 10	As calculated by Release equation 10	As calculated by Release equation 10
RECEPTORS AND PATHWAYS					
Terrestrial receptors					
$PEC_{soil} = \frac{Q}{A \times d \times \rho_s} \times 10^6$	$\boldsymbol{PEC_{soil}}$	**Chemical concentration in the receiving terrestrial environment (mg/kg)**	**Exposure equation 4**	**Exposure equation 4**	**Exposure equation 4**
	$Q = Q$ calculated for each point of release	Quantity of chemical released (kg or L)	As calculated by Input equation 1	As calculated by Input equation 1	As calculated by Input equation 1
	A	Spill area (m^2)	As calculated by Exposure equation 6	As calculated by Exposure equation 6	As calculated by Exposure equation 6A
	d	Depth of penetration (m) [12]	0.02	0.1	0.1
	ρ_s	Soil bulk density (kg/m^3) [13]	1500	1500	1500
$A = {}^{V_T}/_{h}$	$\boldsymbol{A}$	**Area of the spill for liquids (m^2)**	**Exposure equation 6**	**Exposure equation 6**	**Exposure equation 6**
	V_T	Chemical volume spilled (m^3)	Bounding estimate values from Table B.2 to Table B.35	High-end estimate values from Table B.2 to Table B.35	N/A
	h	Height of spill (m)	As calculated by Exposure equation 5	As calculated by Exposure equation 5	N/A
$A = {}^{V_T}/_{\rho_f}$	$\boldsymbol{A}$	**Area of the spill for solid (m^2)**	**Exposure equation 6A**	**Exposure equation 6A**	**Exposure equation 6A**
	V_T	Formulation volume (kg)	N/A	N/A	Central tendency estimate values from Table B.2 to Table B.35

[12] 1-20 cm depth of soil (DoEE 2017) to which contaminants may penetrate.
[13] Several publications (US EPA 2005a, 2005b; EPHC 2009) have separately determined default values for the density of soil based on averages of measured values (1 500 kg/m^3).

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
	ρ_f	Solid formulation density (kg/m^3)	N/A	N/A	Chemical dependent
$h = \sqrt{\frac{(1 - cos(\beta) \times \sigma}{\rho \times g}}$	$\boldsymbol{h}$	**Height of the spill (cm)**	**Exposure equation 5**	**Exposure equation 5**	**Exposure equation 5**
	β	Contact angle [14]	30	30	30
	σ	Soil surface tension (g.cm/s^2) [15]	140	140	140
	ρ	Liquid density (g/cm^3) [16]	Assumed value = 1	Assumed value = 1	Assumed value = 1
	g	Gravitational acceleration (cm/s^2)	980	980	980
Indirect release – During irrigation and dust suppression					
$PEC_{soil_edge} = (W \times\times 1000)/(d \times \rho)$	$\boldsymbol{PEC_{soil_edge}}$	**Soil predicted environmental concentration at the edge of field (mg/kg)**	**Release equation 11**	**Release equation 11**	**Release equation 11**
	W	Chemical application rate (g/m^2/y)	As calculated by Release equation 12	As calculated by Release equation 12	As calculated by Release equation 12
	d	Soil mixing depth (m)	0.02	0.1	0.1
	ρ	Soil bulk density (kg/m^3)	1500	1500	1500
$W = A \times C_{irrigation}$	$\boldsymbol{W}$	**Chemical application rate (g/m^2)**	**Input equation 12**	**Input equation 12**	**Input equation 12**
	A	Application rate of wastewater containing hydraulic fracturing chemicals for irrigation (L/m^2)	1000/y	1000/y	100/irrigation event
	$C_{irrigation}$	Concentration of a chemical in wastewater dam (g/L)	As calculated by Release equation 10	As calculated by Release equation 10	As calculated by Release equation 10
Aquatic receptors					
			Tier 1 uses lower bound estimates to represent typical Australia-wide values for area, receiving volume and rainfall-runoff characteristics	Tier 2 uses upper bound values as determined from maps of the bioregion and historic streamflow and rainfall records	Tier 3 uses lower, central tendency and upper bound values as determined from maps of the bioregion and historic streamflow and rainfall records
$V_{water} = V_{environmental} + V_{contaminated} + V_{uncontaminated}$	$\boldsymbol{V_{water}}$	**Volume of environmental aquatic receptor (L)**	**Exposure equation 3**	**Exposure equation 3**	**Exposure equation 3**
	$V_{environmental}$	Volume of environmental aquatic receptor (L)	1 500 000	6 700 000 [17]	21 000 000–373 000 000 [18]

[14] 30º is a reasonable value for a hydrophilic liquid spill or a hydrophilic surface. The contact angle will increase with a more hydrophilic surface, with an associated increase in height, but smaller area.
[15] 140–205 g cm/s^2 for very low permeable soil.
[16] 1 g/cm^3, assuming most chemicals are hydrophilic.
[17] This value was calculated by estimating the 25th percentile of mean daily flows > 1.5 ML/d over 30 years of data for bioregional rivers and selecting the lowest flow river in a bioregion sub-region.
[18] This used lower, intermediate and upper values. Calculated by estimating the minimum, median and maximum of mean daily values > 6.7 ML/d over 30 years of data for rivers near the working site.

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
	Direct release – $V_{contaminated}$	Volume of drilling and hydraulic fracturing fluid released into the aquatic receptor (L)	V	V	V
	– V	Formulation volume spilled (L)	Bounding estimate from industry data	High-end estimate from industry data	Central tendency estimate from industry data
	Indirect release – $V_{contaminated}$	Volume of drilling and hydraulic fracturing fluid released into the terrestrial receptor (L)	A x R x L%runoff	A x R x L%runoff	A x R x L%runoff
	A	Runoff area (m^2)	As calculated by Exposure equation 6	As calculated by Exposure equation 6	As calculated by Exposure equation 6
	R	Runoff volume (mm/day)	As calculated by Exposure equation 14 (see below under 'Runoff')	As calculated by Exposure equation 14 (see below under 'Runoff')	As calculated by Exposure equation 14 (see below under 'Runoff')
	– $L\%_{runoff}$	Fraction of chemical in runoff water (%)	As calculated by Exposure equation 9 (see below under 'Runoff')	As calculated by Exposure equation 9 (see below under 'Runoff')	As calculated by Exposure equation 9 (see below under 'Runoff')
	Direct release – $V_{uncontaminated}$	Volume of uncontaminated water (L)	0	N/A	N/A
	Indirect release – $V_{uncontaminated}$	Volume of uncontaminated water (L)	0	A x R x L%runoff (A is tenement area)	A x R x L%runoff (A is tenement area)
$PEC_{aquatic} = \frac{\mathrm{Q}}{\mathrm{V_{Water}}} \times 10^6\ \mathrm{mg/L}$	$\boldsymbol{PEC_{aquatic}}$	**Predicted environmental concentration in the aquatic receptor (mg/L)**	**Exposure equation 1**	**Exposure equation 1**	**Exposure equation 1**
	Direct release – Q	Chemical quantity loaded directly to water from each point of release	As calculated by Release equation 1	As calculated by Release equation 1	As calculated by Release equation 1
	Indirect release Q_R	Chemical quantity loaded to water after runoff	As calculated by Release equation 1A (see below under 'Runoff')	As calculated by Release equation 1A (see below under 'Runoff')	As calculated by Release equation 1A (see below under 'Runoff')
	– V_{Water}	Volume of environmental aquatic receptor (L)	As calculated by Exposure equation 3	As calculated by Exposure equation 3	As calculated by Exposure equation 3
– $PEC_{aquaticIrrOrDustS} = (Q_{irrigatiIrrOrDustS} \times 10)/((V_{contaminated} \times 10) + V_{uncontiminated} + V_{environmental})$	$\boldsymbol{PEC_{aquaticIrr\&DustS}}$	**Predicted environmental concentration in the aquatic receptor from irrigation (mg/L)**	**Exposure equation 1B**	**Exposure equation 1B**	**Exposure equation 1B**
	$Q_{irrigatiIrrOrDustS} \times 10$	Quantity of chemical applied to 10 ha via irrigation (mg/L)	As calculated by Release equation 14 (see previous under 'Irrigation and dust suppression')	As calculated by Release equation 14 (see previous under 'Irrigation and dust suppression')	As calculated by Release equation 14 (see previous under 'Irrigation and dust suppression')
	$V_{contaminated} \times 10$	Volume of contaminated water running off from 10 ha (equivalent to rainfall volume across x ha) (L)	Calculated for 10 ha area	Calculated for 10 ha area	Calculated for 10 ha area
	$V_{contaminated}$	Volume of uncontaminated water (L)	0	See inputs to Exposure equation 3	See inputs to Exposure equation 3
	$V_{environment}$	Volume of environmental aquatic receptor (L)	See inputs to Exposure equation 3	See inputs to Exposure equation 3	See inputs to Exposure equation 3

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
$K_{airwater} = H/RT$	$\boldsymbol{K_{airwater}}$	**Air-water partition coefficient (unitless)**	**N/A**	**N/A**	**Exposure equation 19**
	H	Henry's Law Constant (Pa m^3/mol)	N/A	N/A	Varies as chemical specific [19]
	R	Gas constant (J/K mol)	N/A	N/A	8.31
	T	Absolute temperature in Kelvin (K)	N/A	N/A	298
$PEC_{air} = K_{airwater} \times PEC_{aquatic}$	$\boldsymbol{PEC_{air}}$	**Concentration of chemical volatilised from the water column (g/L)**	**N/A**	**N/A**	**Exposure equation 20**
	$K_{airwater}$	Air-water partition coefficient (unitless)	N/A	N/A	As calculated by Exposure equation 19
	$PEC_{aquatic}$	Predicted environmental concentration in the aquatic ecosystem and / or watercourse (g/L)	N/A	N/A	As calculated by Exposure equation 1
– $K_{sediment_water} = 0.8 + (0.2 \times {K_d}/{1000}) \times \rho_{solid}$	$\boldsymbol{K_{sediment_water}}$	**Solid-water partition coefficient in sediment (unitless)**	**N/A**	**N/A**	**Exposure equation 21**
	K_d	The water soil partitioning coefficient (L/kg)	N/A	N/A	Varies as chemical specific (assume the chemical is soluble if data isn't available)
	– ρ_{solid}	Bulk density of solid phase only (kg/m^3)	N/A	N/A	Assumed = 2 400 kg/m^3 or a central tendency value
– $PEC_{sediment} = {K_{sediment_water}}/{\rho_{sediment}} \times$	$\boldsymbol{PEC_{sediment}}$	**Predicted environmental concentration in sediment (mg/kg)**	**N/A**	**N/A**	**Exposure equation 22**
	$K_{sediment_water}$	Solid-water partition coefficient in sediment	N/A	N/A	As calculated by Exposure equation 21
	PEC_{water}	Predicted environmental concentration in water (mg/L)	N/A	N/A	As calculated by Exposure equation 1
	$\rho_{sediment}$	Bulk density of sediment including pore water (kg/m^3)	N/A	N/A	Assumed = 1 280 kg/m^3 or a central tendency value
$PEC_{edgeoffield} = Q_{irrigationOrDustS}/V_{contaminated}$	$\boldsymbol{PEC_{edgeoffield}}$	**Contaminant concentration at the edge of field after irrigation/dust suppression (g/L)**	**Release equation 13**	**Release equation 13**	**Release equation 13**
	$Q_{irrigationOrDustS}$	Quantity of chemical applied to area via irrigation (g)	As calculated by Release equation 14 (for 1 ha)	As calculated by Release equation 14 (for 1 ha)	As calculated by Release equation 14 (for 1 ha)
	$V_{contaminated}$	Volume of contaminated water running off from area (equivalent to rainfall volume across given area) (L)	As calculated by Release equation 14 (for 1 ha)	As calculated by Release equation 14 (for 1 ha)	As calculated by Release equation 14 (for 1 ha)

[19] Values are reported in Table A.13 and Table A.14 of this report. It was assumed that the chemical is not volatile (i.e. = 0) if data were not available.

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
Runoff					
$\mathrm{Q_R} = Q\ x\ L\%_{runoff}$	$\mathbf{Q_R}$	**Quantity of chemical released in the runoff (kg)**	**Release equation 1A**	**Release equation 1A**	**Release equation 1A**
	Q	Quantity of chemical released from each point of release (kg or L)	As calculated by Input equation 1	As calculated by Input equation 1	As calculated by Input equation 1
	$L\%_{runoff}$	Fraction of chemical in runoff water (%)	As calculated by Exposure equation 9	As calculated by Exposure equation 9	As calculated by Exposure equation 9
$L\%_{runoff} = (R/\Psi) \times Cr_{soil_surface} \times f1slope \times f2bufferzone \times f3foliar_application \times heterogeneity_factor \times 100^{\circ} + suspended_contaminant_{\%}$	$\boldsymbol{L\%_{runoff}}$	**Fraction of chemical in runoff water (%)**	**Exposure equation 9**	**Exposure equation 9**	**Exposure equation 9**
	– R	Runoff volume (mm/day) – rainfall is converted to inches to calculate runoff in inches, then converted to mm	As calculated by Exposure equation 14 (see below)	As calculated by Exposure equation 14 (see below)	As calculated by Exposure equation 14 (see below)
	– Ψ	Rainfall (mm/day)	30	30	3–6 [20]
	$Cr_{soil_surface}$	Variable dependent on chemical degradation kinetics and soil adsorption	N/A	As calculated by Exposure equation 10 (see below)	As calculated by Exposure equation 10 (see below)
	– $f1slope$	Variable dependent on slope	As calculated by Exposure equation 11 (see below)	As calculated by Exposure equation 11 (see below)	As calculated by Exposure equation 11 (see below)
	$f2bufferzone$	Filtering buffer variable	Assumed value = 1	Assumed value = 1	0.024 [21]
	$f3foliar_application$	Parameter dependent on interception and retention by foliage	Assumed value = 1 (see Exposure equation 13)	Assumed value = 1	0.75 [22]
	$heterogeneity_factor$	Variable allowing for partial area runoff [23]	Assumed value = 1	Assumed value = 1	Assumed value = 0.5
	$suspended_contaminant_{\%}$	Contaminant adsorbed to particulates and held in suspension	Assumed value = 0	Assumed value = 0	Assumed value = 0
$R = (\Psi - 0.2S)^2/(\Psi + 0.8S)$	$\boldsymbol{R}$	**Runoff volume (mm/day) – rainfall is converted to inches to calculate runoff in inches, then converted to mm**	**Exposure equation 14**	**Exposure equation 14**	**Exposure equation 14**
	Ψ	Rainfall (mm/day)	30	30	3–6 [24]
	S	Maximum potential retention	Calculated from CN	Calculated from CN	Calculated from CN

[20] Values vary from 3 to 6 mm/day over the five work sites assessed.
[21] Calculated from Exposure equation 12 for f2buffer_zone. Assumed conservative value of 20 m at Tier 3.
[22] Calculated from Exposure equation 13 for f3foliar_application. Assumed F_{int} = 0.5 to account for all stages of vegetation life cycle.
[23] Set between > 0 and < 1.
[24] Values vary from 3 to 6 mm/day over the five work sites assessed.

Equations	Variable	Variable description	Tier 1 – Generic assessment	Tier 2 – Regional assessment	Tier 3 – Site specific assessment
	CN	Curve number [25]	90	Assumed value = 90	Assumed value = 90
$f1slope$ $= 0.02153 \times slope + 0.001423$ $\times slope^2 for\ slope < 20\%;$ $= 1\ for\ slope \geq 20\%$	$\boldsymbol{f1slope}$	**Variable dependent on slope**	**Exposure equation 11**	**Exposure equation 11**	**Exposure equation 11**
	$slope$	Slope of land over which water runs off in % [26]	12.5	9	7
$f2bufferzone = 0.83^{buffer\ width}$	$\boldsymbol{f2bufferzone}$	**Buffer zone filter factor**	**Exposure equation 12**	**Exposure equation 12**	**Exposure equation 12**
	buffer width (m)	Width of buffer zone able to filter chemicals from runoff water (m)	Assumed value = 0	Assumed value = 0	Conservative value = 20
$f3foliar_application$ $= 1 - F_{int} \times 0.5$	$\boldsymbol{f3foliar_application}$	**Foliage retention factor**	**Exposure equation 13**	**Exposure equation 13**	**Exposure equation 13**
	F_{int}	Fraction of chemical intercepted by foliage	0 [27]	Assumed value = 0	Assumed value = 0.5
$Cr_{soil_surface}$ $= e^{(-3 \ln 2/DT50soil)} \times [1/(1 + K_d)]$	$\boldsymbol{Cr_{soil_surface}}$	**Variable dependent on chemical degradation kinetics and soil adsorption**	**N/A**	**Exposure equation 10**	**Exposure equation 10**
	$DT50soil$	Soil degradation half-life	Assumption = no degradation	Varies as chemical dependent [28]	Varies as chemical dependent (as per Tier 2)
	Kd	Water soil partitioning coefficient	N/A (assumed value = 0)	As calculated from Exposure equation 15	Calculated from Exposure equation 15
$Kd = Koc \times \%OC/100$	$\boldsymbol{Kd}$	**Water soil partitioning coefficient**	**Assumption = water soluble (value = 0)**	**Exposure equation 15**	**Exposure equation 15**
	Koc	Water organic partitioning coefficient	N/A	Varies as chemical dependent [29]	Varies as chemical dependent (as per Tier 2)
	$\%OC$	Weight % of organic carbon in soil	N/A	1 [30]	1 [31]

[25] The CN is based on soils, plant cover, amount of impervious areas, interception and surface storage, and its value can be used to calculate the volume of runoff from a certain volume of rain. Ninety (90) is used for gravel and dirt roads and open spaces in poor condition (USDA 1986).
[26] 20%, 12.5%, 9%, 7.5% or 5% (Balmer & Frey 2001; OECD 2000) and available GIS data or ASRIS database CSIRO (2013) for each region.
[27] For bare soil (Linders et al. 2000).
[28] Values reported in Table A.13 and Table A.14 of this report. It was assumed that chemical is not degradable (i.e. = 0) if data were not available.
[29] Values reported in Table A.13 and Table A.14 of this report. It was assumed that chemical is not soluble (i.e. = 0) if data were not available.
[30] Values from regional %OC data available in ASRIS database (CSIRO 2013).
[31] Values from regional %OC data available in ASRIS database (CSIRO 2013).

1.4 Industry data (treated)

Industry data was provided in 2015 to inform th
concentrations of chemicals used at working si
the assessment, well site data for five operatin
intermediate storage facility. Treated data is pr
life-cycle, where applicable.

1.4.1 Working Site 1

Tables of the treated data for Working Site 1, c
on the following pages. In summary, for drilling

- data were provided for transport from wa
- transport from intermediate storage to W
  six chemicals listed
- where there were data gaps, substitute v
  (NIC) Bioregion were adopted. These we
  where only one other company used a pa
  substitute company's well sites
- no injection volume or diluted concentrati
  volumes of injection fluid from the NIC Bi
  concentrations were then back calculated

For the hydraulic fracturing chemicals:

- all transport volumes and concentrations
- no intermediate storage data were report
  transported directly from Supplier Wareh
- no formulations were transported to Well
  required on-site
- two injection fluid mixtures were used an
  Site. Diluted concentrations were calcula
  well. The average was then taken across

Table B.2 Drilling chemical concentrations and volu

Work Site 1 – Drilling	
CAS RN	***Chemical***
11138-66-2	Xanthan gum

Work Site 1 – Drilling			**Transport volume (Intermediate Storage to Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	
1310-73-2	Sodium hydroxide (Na(OH))	L	3125	800	200	980
497-19-8	Carbonic acid, disodium salt	S	25	25	25	970
7447-40-7	Potassium chloride (KCl)	S	28800	9205	7135	970
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	20000	280	63	990
CBI	Polymer with substituted alkylacrylamide salt	S	25	25	25	900

Table B.3 Drilling chemical concentrations and volumes for Intermediate Storage – Working Site 1

Work Site 1 – Drilling			**Storage volume (Intermediate)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	
11138-66-2	Xanthan gum	S	1800	1800	625	870
497-19-8	Carbonic acid, disodium salt	S	1050	1050	925	970
7447-40-7	Potassium chloride (KCl)	S	8400	8400	2475	970
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	1125	1125	950	990
CBI	Polymer with substituted alkylacrylamide salt	S	950	950	850	900

Table B.4 Drilling chemical concentrations and volumes for Well Storage – Working Site 1

Work Site 1 – Drilling			**Storage volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
11138-66-2	Xanthan gum	S	175	175	75	870
1310-73-2	Sodium hydroxide (Na(OH))	L	1450	1450	1450	999.9
497-19-8	Carbonic acid, disodium salt	S	50	50	25	970
7447-40-7	Potassium chloride (KCl)	S	9450	9205	7135	990
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	1000	910	550	999
CBI	Polymer with substituted alkylacrylamide salt	S	25	25	25	900

Table B.5 Drilling chemical concentrations and volumes for Well Use – Working Site 1

Work Site 1 – Drilling			**Used volume (Well Site)**	**Chemical concentration**	**Injected volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (kg)***	***C_{fmax} (g/kg)***	***V_U (L)***			***C_D (g/L)***
			(Solid, kg)	***(Solid, kg)***	***Max***	***High-end***	***Average***	***Max***
11138-66-2	Xanthan gum	L	1175	870	160000	160000	115000	6.4
1310-73-2	Sodium hydroxide (Na(OH))	L	175	980	160000	160000	115000	1.1
497-19-8	Carbonic acid, disodium salt	L	125	970	160000	160000	115000	0.8
7447-40-7	Potassium chloride (KCl)	L	5875	970	160000	160000	115000	35.6
77-92-9	1,2,3-Propanetricarbo	L	175	990	160000	160000	115000	1.1

Work Site 1 – Drilling			**Used volume (Well Site)**	**Chemical concentration**	**Injected volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (kg)***	***C_{fmax} (g/kg)***	***V_U (L)***			***C_D (g/L)***
			(Solid, kg)	***(Solid, kg)***	***Max***	***High-end***	***Average***	***Max***
	xylic acid, 2-hydroxy-							
CBI	Polymer with substituted alkylacrylamide salt	L	100	900	160000	160000	115000	0.6

Table B.6 Hydraulic fracturing chemical concentrations and volumes for Transport – Working Site 1

Work Site 1 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Storage to Well Site)**			**Chemical concentration**		
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***		
			Max	***High-end***	***Average***	***Max***	***High-end***	***Average***
1310-73-2	Sodium hydroxide (Na(OH))	L	2006	2006	2006	500	500	500
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	640	640	470	750	705	300
64-19-7	Acetic acid	L	5016	5016	5016	600	600	600
7647-01-0	Hydrochloric acid	L	9000	9000	5000	320	320	320
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	998	998	998	1000	1000	1000
9000-30-0	Guar gum	S	5850	5850	4725	1000	1000	1000

Table B.7 Hydraulic fracturing chemical concentrations and volumes for Intermediate Storage – Working Site 1

Work Site 1 – Hydraulic fracturing			**Storage (Intermediate)**			**Chemical concentration**		
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***		
			Max	***High-end***	***Average***	***Max***	***High-end***	***Average***
1310-73-2	Sodium hydroxide (Na(OH))	L	N/A	N/A	N/A	N/A	N/A	N/A
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	N/A	N/A	N/A	N/A	N/A	N/A
64-19-7	Acetic acid	L	N/A	N/A	N/A	N/A	N/A	N/A
7647-01-0	Hydrochloric acid	L	N/A	N/A	N/A	N/A	N/A	N/A
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	N/A	N/A	N/A	N/A	N/A	N/A
9000-30-0	Guar gum	S	N/A	N/A	N/A	N/A	N/A	N/A

Table B.8 Hydraulic fracturing chemical concentrations and volumes for Well Storage – Working Site 1

Work Site 1 – Hydraulic fracturing			**Storage volume (Well Site)**			**Chemical concentration**		
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***		
			Max	***High-end***	***Average***	***Max***	***High-end***	***Average***
1310-73-2	Sodium hydroxide (Na(OH))	L	2006	2006	1956	500	500	500
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	661	661	258	750	705	300
64-19-7	Acetic acid	L	5016	5016	4729	600	600	600
7647-01-0	Hydrochloric acid	L	9029	9029	4881	320	320	320
77-92-9	1,2,3-Propanetricarboxylic	S	998	998	758	1000	1000	1000

Work Site 1 – Hydraulic fracturing			Storage volume (Well Site)			Chemical concentration		
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***		
			Max	***High-end***	***Average***	***Max***	***High-end***	***Average***
	acid, 2-hydroxy-							
9000-30-0	Guar gum	S	5635	5635	3148	1000	1000	1000

Table B.9 Hydraulic fracturing chemical concentrations and volumes for Well Use – Working Site 1

Work Site 1 – Hydraulic fracturing			Injection volume (Well Site Use)			Chemical concentration		
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (L)***			***C_{fmax} (g/kg)***		
			Max	***High-end***	***Average***	***Max***	***High-end***	***Average***
1310-73-2	Sodium hydroxide (Na(OH))	L	810415	810415	810415	0.021	0.021	0.021
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	810415	810415	810415	0.138	0.138	0.090
64-19-7	Acetic acid	L	810415	810415	810415	0.055	0.055	0.120
7647-01-0	Hydrochloric acid	L	810415	810415	810415	1.156	1.156	1.019
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	L	810415	810415	810415	0.226	0.226	0.159
9000-30-0	Guar gum	L	810415	810415	810415	2.78	2.78	1.81

1.4.2 Working Site 2

Tables of the treated data for Working Site 2, drilling and hydraulic fracturing, are presented on the following pages. In summary, for drilling chemicals:

- no data were provided.

For the hydraulic fracturing chemicals:

- two chemicals were reported

- reported to be transported directly from Supplier Warehouse to Well Site, with the first Well Site acting as an 'Intermediate Storage'.

Table B.10 Hydraulic fracturing chemical concentrations and volumes for Transport – Working Site 2

Work Site 2 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Storage to Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	650	650	650	600
64-19-7	Acetic acid	L	2000	2000	2000	600

Table B.11 Hydraulic fracturing chemical concentrations and volumes for Intermediate Storage – Working Site 2

Work Site 2 – Hydraulic fracturing			**Storage volume (Intermediate)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	195	140	130	600
64-19-7	Acetic acid	L	2000	2000	1500	600

Table B.12 Hydraulic fracturing chemical concentrations and volumes for Well Storage – Working Site 2

Work Site 2 – Hydraulic fracturing			**Storage volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	195	140	130	600
64-19-7	Acetic acid	L	2000	2000	1500	600

Table B.13 Hydraulic fracturing chemical concentrations and volumes for Well Use – Working Site 2

Work Site 2 – Hydraulic fracturing			**Injection volume (Use)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	932 051	932 051	932 051	0.31
64-19-7	Acetic acid	L	932 051	932 051	932 051	0.31

1.4.3 Working Site 3

Tables of the treated data for Working Site 3, drilling and hydraulic fracturing, are presented on the following pages. In summary, for drilling chemicals:

- five chemicals were reported
- no volume data were provided for transport, storage or use. Substitute values from the NIC Bioregion were adopted. Generally, these were values averaged across all working sites, or where only one other company used a particular chemical, averaged across the substitute company's Well Sites. Where the company was the only reported user at the well site, transport and storage volumes were derived from Supplier's Intermediate Storage facility
- no injection volume data were provided. Diluted concentrations were provided. Where possible, the injection volume was back calculated from the diluted concentration and

assumptions over the quantities stored and used. Substitute data from the NIC bioregion was also used if the calculations produced unrealistic values.

For the hydraulic fracturing chemicals:

- no Intermediate Storage for reported chemicals. Chemicals transported directly from Supplier Warehouse to Well Site
- Well Sites were grouped into areas A, B and C.

Table B.14 Drilling chemical concentrations and volumes for Transport – Working Site 3

Working Site 3 – Drilling			**Transport volume (Warehouse or Intermediate Storage to Well Site)**		**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***		***C_{fmax} (g/kg)***
			High-end	***Average***	***Max***
111-30-8	Pentanedial/Glutaraldehyde	L	927	927	300
11138-66-2	Xanthan gum	S	990	875	1000
144-55-8	Carbonic acid, monosodium salt	S	612	612	1000
497-19-8	Carbonic acid, disodium salt	S	550	550	1000
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	280	63	1000

Table B.15 Drilling chemical concentrations and volumes for Well Storage – Working Site 3

Working Site 3 – Drilling			**Storage volume (Well Site)**		**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***		***C_{fmax} (g/kg)***
			High-end	***Average***	***Max***
111-30-8	Pentanedial/Glutaraldehyde	L	927	244	300
11138-66-2	Xanthan gum	S	1990	1550	1000
144-55-8	Carbonic acid, monosodium salt	S	612	207	1000
497-19-8	Carbonic acid, disodium salt	S	550	550	1000
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	910	550	1000

Table B.16 Drilling chemical concentrations and volumes for Well Use – Working Site 3

Working Site 3 – Drilling			**Injection volume (Use)**		**Chemical concentration**	
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (L)***		***C_U (g/L)***	
			High-end	***Average***	***High-end***	***Average***
111-30-8	Pentanedial/Glutaraldehyde	L	42513	42513	6.5	3.2
11138-66-2	Xanthan gum	L	235079	143355	3.8	3.6
144-55-8	Carbonic acid, monosodium salt	L	243348	243348	2.5	0.6
497-19-8	Carbonic acid, disodium salt	L	160000	115000	7.8	4.4
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	L	367710	252895	4.0	2.5

Table B.17 Hydraulic fracturing chemical concentrations and volumes for Transport – Working site 3

Work Site 3 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Storage to Well Site), V_T (kg)**									**Chemical concentration, C_{fmax} (g/kg)**		
CAS RN	***Chemical***	***State (solid or liquid)***	***Max***			***High-end***			***Average***			***Max***		
			A	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***
1310-73-2	Sodium hydroxide (Na(OH))	L	120	120	1000	120	120	760	24	24	760	20	20	500
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	S	75			75			45			100		
2682-20-4	3-Isothiazolone, 2-methyl-	S	37.5			37.5			22.5			50		
64-19-7	Acetic acid	L	5000	5000	2000	5000	5000	2000	3500	3000	2000	600	600	600
7447-40-	Potassium	S			27			27			22			1

Work Site 3 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Storage to Well Site), V_T (kg)**									**Chemical concentration, C_{fmax} (g/kg)**		
CAS RN	***Chemical***	***State (solid or liquid)***	***Max***			***High-end***			***Average***			***Max***		
			A	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***
7	chloride (KCl)				000			000			500			000
7647-01-0	Hydrochloric acid	L			11000			11000			2000			320

Table B.18 Hydraulic fracturing chemical concentrations and volumes for Well Storage – Working Site 3

Work Site 3 – Hydraulic fracturing			**Storage volume (Well Site), V_T (kg)**									**Chemical concentration, C_{fmax} (g/kg)**		
CAS RN	***Chemical***	***State (solid or liquid)***	***Max***			***High-end***			***Average***			***Max***		
			A	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***
1310-73-2	Sodium hydroxide (Na(OH))	L	120	120	760	120	120	760	24	24	760	20	20	500
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	S	75			75			45			100		
2682-20-4	3-Isothiazolone, 2-methyl-	S	37.5			37.5			22.5			50		
64-19-7	Acetic acid	L	5000	5000	2000	5000	5000	2000	3500	3000	1000	600	600	600
7447-40-7	Potassium chloride (KCl)	S			45000			45000			27000			1000
7647-01-0	Hydrochloric acid	L			11000			9000			6000			320

Table B.19 Hydraulic fracturing chemical volumes for Well Use – Working Site 3

Work Site 3 – Hydraulic fracturing			**Injection volume (Use), V_U (L)**								
CAS RN	***Chemical***	***State (solid or liquid)***	***Max.***			***High-end***			***Average***		
			A	***B***	***C***	***A***	***B***	***C***	***A***	***B***	***C***
1310-73-2	Sodium hydroxide (Na(OH))	L		2012526	1083957		1746626	1083957	808331	12276600	1083957
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	L	1379121			965237			808331		
2682-20-4	3-Isothiazolone, 2-methyl-	L	1379121			965237			808331		
64-19-7	Acetic acid	L	1379121	2012526	1083957	965237	1746626	1083957	808331	12276600	1083957
7447-40-7	Potassium chloride (KCl)	L			1083957			1083957			1083957
7647-01-0	Hydrochloric acid	L			1083957			1083957			1083957

Table B.20 Hydraulic fracturing chemical concentrations for Well Use – Working Site 3

Work Site 3 – Hydraulic fracturing			**Chemical concentration, C_U (g/L)**		
CAS RN	***Chemical***	***State (solid or liquid)***	***Max***		
			A	***B***	***C***
1310-73-2	Sodium hydroxide (Na(OH))	L	0.021	0.021	0.00016
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	L	0.00377		
2682-20-4	3-Isothiazolone, 2-methyl-	L	0.00116		
64-19-7	Acetic acid	L	0.285	0.309	0.00085
7447-40-7	Potassium chloride (KCl)	L			0.0028

Work Site 3 – Hydraulic fracturing			**Chemical concentration, C_U (g/L)**		
CAS RN	***Chemical***	***State (solid or liquid)***	***Max***		
			A	***B***	***C***
7647-01-0	Hydrochloric acid	L			0.89

1.4.4 Working Site 4

Tables of the treated data for Working Site 4, drilling and hydraulic fracturing, are presented on the following pages. In summary, for drilling chemicals:

- six listed chemicals were reported
- volume and concentration data were provided for chemicals used at a typical Well Site and also Well Sites identified within 2 km of an aquatic receptor
- this typical data were included for Tier 1 and Tier 2 assessments to provide a better dataset for the bioregion, while Tier 3 assessment focused on specific Well Sites within 2 km of an aquatic receptor.

For the hydraulic fracturing chemicals:

- all transport volumes and concentrations provided for reported chemicals during transport and storage at the well site
- no Intermediate Storage for reported chemicals. Chemicals transported directly from Supplier Warehouse to Well Site
- injection fluid volumes and mixtures differed by well site. The highest, 90th percentile and median values were used in Tier 1, Tier 2 and Tier 3, respectively
- diluted concentrations derived from the percentage (%) fraction of chemical in the injection fluid mixtures and the chemical concentrations for each Well Site. The highest, 90th percentile and median values were used in Tier 1, Tier 2 and 3, respectively.

Table B.21 Drilling chemical concentrations and volumes for Transport – Working Site 4

Work Site 4 – Drilling			**Transport volume (Intermediate Storage to Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
11138-66-2	Xanthan gum*	S	1000	1000	1000	1000
497-19-8	Carbonic acid, disodium salt*	S	550	550	550	600
7447-40-7	Potassium chloride (KCl)	S	7000	7000	4820	990

Work Site 4 – Drilling			**Transport volume (Intermediate Storage to Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-*	S	100	100	100	980
7647-14-5	Sodium chloride (NaCl)*	S	1200	1200	1200	990
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)*	L	175	175	175	250

** Chemical used at a 'typical' well site. It is not reported for well sites identified near to an aquatic receptor.*

Table B.22 Drilling chemical concentrations and volumes for Intermediate Storage – Working Site 4

Work Site 4 – Drilling			**Storage volume (Intermediate)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
11138-66-2	Xanthan gum*	S	1500	1500	1500	1000
497-19-8	Carbonic acid, disodium salt*	S	660	660	660	600
7447-40-7	Potassium chloride (KCl)	S	200000	200000	150000	990
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-*	S	60	60	60	980
7647-14-5	Sodium chloride (NaCl)*	S	2880	2880	2880	990
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)*	L	210	210	210	250

***** Chemical used at a 'typical' well site. It is not reported for well sites identified near to an aquatic receptor.

Table B.23 Drilling chemical concentrations and volumes for Well Storage – Working Site 4

Work Site 4 – Drilling			**Storage volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
11138-66-2	Xanthan gum*	S	1000	1000	1000	1000
497-19-8	Carbonic acid, disodium salt*	S	550	550	550	600
7447-40-7	Potassium chloride (KCl)	S	7000	7000	4820	990
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-*	S	100	100	100	980
7647-14-5	Sodium chloride (NaCl)*	S	1200	1200	1200	990
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)*	L	175	175	175	250

Table B.24 Drilling chemical concentrations and volumes for Well Use – Working Site 4

Work Site 4 – Drilling			**Injected volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (L)***			***C_D (g/L)***
			Max (QGC)	***High-end (QGC)***	***Average (QGC)***	***Max***
11138-66-2	Xanthan gum*	L	160000	160000	115000	3.566
497-19-8	Carbonic acid, disodium salt*	L	160000	160000	115000	8.56
7447-40-7	Potassium chloride (KCl)	L	160000	160000	115000	160
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-*	L	160000	160000	115000	4.19
7647-14-5	Sodium chloride (NaCl)*	L	160000	160000	115000	127.1

Work Site 4 – Drilling			**Injected volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (L)***			***C_D (g/L)***
			Max (QGC)	***High-end (QGC)***	***Average (QGC)***	***Max***
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)*	L	160000	160000	115000	3.57

* Chemical used at a 'typical' well site. It is not reported for well sites identified near to an aquatic receptor.

Table B.25 Hydraulic fracturing chemical concentrations and volumes for Transport – Working Site 4

Work Site 4 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Storage to Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Ma	***High-end***	***Average***	***Max***
107-21-1	1,2-Ethanediol*	L	1000	1000	1000	400
111-76-2	Ethanol, 2-butoxy-*	L	208	208	208	600
1310-73-2	Sodium hydroxide (Na(OH))*	L	208	208	208	300
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	S	41	41	36	100
2682-20-4	3-Isothiazolone, 2-methyl-	S	20.5	20.5	18	50
7447-40-7	Potassium chloride (KCl)*	S	13200	13200	13200	1000
7647-01-0	Hydrochloric acid	L	1000	1000	1000	320
7647-14-5	Sodium chloride (NaCl)*	L	196	196	196	1000**
7727-54-0	Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt	S	1180	1180	960	800

Work Site 4 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Storage to Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_T (kg)***			***C_{fmax} (g/kg)***
			Ma	***High-end***	***Average***	***Max***
7786-30-3	Magnesium chloride (MgCl2)	S	41	41	36	100
9000-30-0	Guar gum	S	4362	4362	2908	800
11138-66-2	Xanthan gum*	S	207	207	207	1000**

** Chemical used at a 'typical' well site. It is not reported for well sites identified near to an aquatic receptor.*
*** Confidential Business Information (CBI) and therefore 100% concentration is presented as a worst case assumption.*

Table B.26 Hydraulic fracturing chemical concentrations and volumes for Well Storage – Working Site 4

Work Site 4 – Hydraulic fracturing			**Storage volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
107-21-1	1,2-Ethanediol*	L	1000	1000	1000	400
111-76-2	Ethanol, 2-butoxy-*	L	208	208	208	600
1310-73-2	Sodium hydroxide (Na(OH))*	L	208	208	208	300
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	S	45	45	25	100
2682-20-4	3-Isothiazolone, 2-methyl-	S	22.5	22.5	12.5	50
7447-40-7	Potassium chloride (KCl)*	S	13200	13200	13200	1000
7647-01-0	Hydrochloric acid	L	1000	1000	1000	320
7647-14-	Sodium chloride (NaCl)*	L	196	196	196	1000**

Work Site 4 – Hydraulic fracturing			**Storage volume (Well Site)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max	***High-end***	***Average***	***Max***
5						
7727-54-0	Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt	S	1180	1180	960	800
7786-30-3	Magnesium chloride (MgCl2)	S	45	45	25	100
9000-30-0	Guar gum	S	4362	4362	2908	800
11138-66-2	Xanthan gum*	S	207	207	207	1000**

** Chemical used at a 'typical' well site. It is not reported for well sites identified near to an aquatic receptor.*

*** Confidential Business Information (CBI) and therefore 100% concentration is presented as a worst-case assumption.*

Table B.27 Hydraulic fracturing chemical concentrations and volumes for Well Use – Working Site 4

Work Site 4 – Hydraulic fracturing			**Injection volume (Use)**			**Chemical concentration**		
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (L)***			***C_U (g/kg)***		
			Max	***High-end***	***Average***	***Max***	***High-end***	***Average***
107-21-1	1,2-Ethanediol*	L	618184	618184	618184	0.65	0.65	0.65
111-76-2	Ethanol, 2-butoxy-*	L	618184	618184	618184	0.2	0.2	0.2
1310-73-2	Sodium hydroxide (Na(OH))*	L	618184	618184	618184	0.1	0.1	0.1
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	L	1821574	1511284	1025430	0.001	0.001	0.001
2682-20-4	3-Isothiazolone, 2-methyl-	L	1821574	1511284	1025430	0.00005	0.00005	0.00005
7447-40-7	Potassium chloride (KCl)*	L	618184	618184	618184	21.35	21.35	21.35
7647-01-0	Hydrochloric acid	L	1821574	1511284	1025430	0.32	0.3	0.32
7647-14-5	Sodium chloride (NaCl)*	L	618184	618184	618184	0.32	0.32	0.32
7727-54-0	Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt	L	1821574	1511284	1025430	0.8	0.8	0.8
7786-30-3	Magnesium chloride (MgCl2)	L	1821574	1511284	1025430	0.001	0.001	0.001
9000-30-0	Guar gum	L	1821574	1511284	1025430	8	8	8
11138-66-2	Xanthan gum*	L	618184	618184	618184	0.33	0.33	0.33

** Chemical used at a 'typical' well site. It is not reported for well sites identified near to an aquatic receptor.*

1.4.5 Working Site 5

Tables of the treated data for Working Site 5, drilling and hydraulic fracturing, are presented on the following pages. In summary, for drilling chemicals:

- seven chemicals were reported
- no Intermediate Storage; chemicals are transported directly from Supplier Warehouse or Supplier Intermediate Storage
- Well Sites grouped into areas AB and BB
- no drilling fluid volume information provided
- the maximum injection volume from the NIC bioregion was substituted. Diluted concentrations were subsequently derived from the quantity of chemical transported and stored at the well site.

For the hydraulic fracturing chemicals:

- no Intermediate Storage for reported chemicals. Chemicals are transported directly from Supplier Warehouse to Well Site
- Well Sites grouped into areas AB and BB. The highest, 90th percentile and median values used in Tier 1, Tier 2 and Tier 3, respectively
- injection fluid volumes were provided for each well site
- diluted concentrations were derived from the concentration of each chemical in the stored product and the reported pumping ratios.

Table B.28 Drilling chemical concentrations and volumes for Transport – Working Site 5

Working Site 5 – Drilling			**Transport volume (Warehouse or Intermediate Storage to Well Site), V_T (kg)**												**Chemical Concentration, C_{fmax} (g/kg)**			
CAS RN	***Chemical***	***State (solid or liquid)***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***
			Highest	***Highest***	***Highest***	***Highest***	***High-end***	***High-end***	***High-end***	***High-end***	***Average***	***Average***	***Average***	***Average***	***Max.***	***Max.***	***Max.***	***Max.***
11138-66-2	Xanthan gum	S	1000	900	750	750	1000	900	750	750	1000	900	750	750	1000	1000	1000	1000
1310-73-2	Sodium hydroxide (Na(OH))	L	800	150	200	200	800	150	200	200	800	150	200	200	980	980	980	980
7447-40-7	Potassium chloride (KCl)	S			9450	9450			9450	9450			9450	9450			990	990
7778-80-5	Sulfuric acid, dipotassium salt	S	13000	11300			13000	11300			13000	11300			990	990		
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	25	25	300	300	25	25	300	300	25	25	300	300	990	990	990	990
CBI	Polymer with substituted alkylacrylamide salt	S	25	25			25	25			25	25			990	990		
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	800	120			800	120			800	120			250	250		

Table B.29 Drilling chemical concentrations and volumes for Well Storage – Working Site 5

Working Site 5 – Drilling			**Storage volume (Well Site), V_S (kg)**												**Chemical concentration, C_{fmax} (g/kg)**			
CAS RN	***Chemical***	***State (solid or liquid)***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***
			Highest	***Highest***	***Highest***	***Highest***	***High-end***	***High-end***	***High-end***	***High-end***	***Average***	***Average***	***Average***	***Average***	***Max.***	***Max.***	***Max.***	***Max.***
11138-66-2	Xanthan gum	S	2100	2000	760	760	2100	2000	760	760	2100	2000	760	760	1000	1000	1000	1000
1310-73-2	Sodium hydroxide (Na(OH))	L	1450	800	200	200	1450	800	200	200	1450	800	200	200	980	980	980	980
7447-40-7	Potassium chloride (KCl)	S			9450	9450			9450	9450			9450	9450			990	990
7778-80-5	Sulfuric acid, dipotassium salt	S	24300	26000			24300	26000			24300	26000			990	990		
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	995	995	995	995
CBI	Polymer with substituted alkylacrylamide salt	S	25	25			25	25			25	25			990	990		
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-,	L	1160	640			1160	640			1160	640			250	250		

Working Site 5 – Drilling			**Storage volume (Well Site), V_S (kg)**												**Chemical concentration, C_{fmax} (g/kg)**			
CAS RN	***Chemical***	***State (solid or liquid)***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***
			Highest	***Highest***	***Highest***	***Highest***	***High-end***	***High-end***	***High-end***	***High-end***	***Average***	***Average***	***Average***	***Average***	***Max.***	***Max.***	***Max.***	***Max.***
	sulfate (2:1) (salt)																	

Table B.30 Drilling chemical concentrations and volumes for Well Use – Working Site 5

Working Site 5 – Drilling			**Injection volume (Use)**		**Chemical concentration**	
CAS RN	***Chemical***	***State (solid or liquid)***	***V_U (L)***		***C_U (g/L)***	
			G3	***G4***	***G7***	***G8***
11138-66-2	Xanthan gum	L	243421	100000	3.8	3.8
1310-73-2	Sodium hydroxide (Na(OH))	L	390789	257895	0.48	0.76
7447-40-7	Potassium chloride (KCl)	L		390789		23.9
7778-80-5	Sulfuric acid, dipotassium salt	L	390789		39.5	
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	L	390789	390789	0.51	0.38
CBI	Polymer with substituted alkylacrylamide salt	L	390789		0.06	
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	390789		0.3	

Table B.31 Hydraulic fracturing chemical concentrations and volumes for Transport – Working site 5

Working Site 5 – Hydraulic fracturing			**Transport volume (Warehouse or Intermediate Site to Well Site), V_T (kg)**												**Chemical concentration, C_{fmax} (g/kg)**			
CAS RN	***Chemical***	***State (solid or liquid)***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***
			Highest	***Highest***	***Highest***	***Highest***	***High-end***	***High-end***	***High-end***	***High-end***	***Average***	***Average***	***Average***	***Average***	***Max.***	***Max.***	***Max.***	***Max.***
10043-35-3	Boric acid (H3BO3)	S	600	600	600	600	600	600	600	600	600	600	600	600	800	800	800	800
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	S	10	10	10	10	10	10	10	10	5	5	5	5	100	100	100	100
2682-20-4	3-Isothiazolone, 2-methyl-	S	5	5	5	5	5	5	5	5	2.5	2.5	2.5	2.5	50	50	50	50
497-19-8	Carbonic acid, disodium salt	S	800	800	800	800	800	800	800	800	800	800	800	800	800	800	800	800
7647-01-0	Hydrochloric acid	L	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	320	320	320	320
7727-54-0	Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt	S	2460	2460	2460	2460	2460	2460	2460	2460	2460	2460	2460	2460	800	800	800	800
7786-30-3	Magnesium chloride (MgCl2)	S	10	10	10	10	10	10	10	10	5	5	5	5	100	100	100	100
9000-30-0	Guar gum	S	2181	2181	2181	2181	2181	2181	2181	2181	2181	2181	2181	2181	800	800	800	800

Table B.32 Hydraulic fracturing chemical concentrations and volumes for Well Storage – Working Site 5

Working Site 5 – Hydraulic fracturing			**Storage volume (Well Site), V_S (kg)**												**Chemical concentration, C_{fmax} (g/kg)**			
CAS RN	***Chemical***	***State (solid or liquid)***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***	***G3***	***G4***	***G7***	***G8***
			Highest	***Highest***	***Highest***	***Highest***	***High-end***	***High-end***	***High-end***	***High-end***	***Average***	***Average***	***Average***	***Average***	***Max.***	***Max.***	***Max.***	***Max.***
10043-35-3	Boric acid (H3BO3)	S	600	600	600	600	600	600	600	600	600	600	600	600	800	800	800	800
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	S	10	10	10	10	10	10	10	10	5	5	5	5	100	100	100	100
2682-20-4	3-Isothiazolone, 2-methyl-	S	5	5	5	5	5	5	5	5	2.5	2.5	2.5	2.5	50	50	50	50
497-19-8	Carbonic acid, disodium salt	S	800	800	800	800	800	800	800	800	800	800	800	800	800	800	800	800
7647-01-0	Hydrochloric acid	L	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	2000	320	320	320	320
7727-54-0	Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt	S	2460	2460	2460	2460	2460	2460	2460	2460	2460	2460	2460	2460	800	800	800	800
7786-30-3	Magnesium chloride (MgCl2)	S	10	10	10	10	10	10	10	10	5	5	5	5	100	100	100	100
9000-30-0	Guar gum	S	2181	2181	2181	2181	2181	2181	2181	2181	2181	2181	2181	2181	800	800	800	800

Table B.33 Hydraulic fracturing chemical concentrations and volumes for Well Use – Working Site 5

Working Site 5 – Hydraulic Fracturing			**Injection volume (Use), V_U (L)**				**Chemical concentration, C_U (g/L)**
CAS RN	***Chemical***	***State (solid or liquid)***	***G3***	***G4***	***G7***	***G8***	
10043-35-3	Boric acid (H3BO3)	L	247400	443700	413200	351500	0.153
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	L	247400	443700	413200	351500	0.0006
2682-20-4	3-Isothiazolone, 2-methyl-	L	247400	443700	413200	351500	0.00015
497-19-8	Carbonic acid, disodium salt	L	247400	443700	413200	351500	0.92
7647-01-0	Hydrochloric acid	L	247400	443700	413200	351500	0.064
7727-54-0	Peroxydisulfuric acid (((HO)S(O)2)2O2), diammonium salt	L	247400	443700	413200	351500	0.307
7786-30-3	Magnesium chloride (MgCl2)	L	247400	443700	413200	351500	0.0006
9000-30-0	Guar gum	L	247400	443700	413200	351500	1.533

1.4.6 Storage Area Working Site 6

Tables of the treated data for Working Site 6 (an intermediate storage facility), drilling and hydraulic fracturing, are presented on the following pages. In summary, for drilling chemicals:

- eight chemicals were reported
- the Intermediate Storage release point was assessed.

For the hydraulic fracturing chemicals:

- eight chemicals were reported
- the Intermediate Storage release point was assessed.

Table B.34 Drilling chemical concentrations and volumes for Intermediate Storage – Working Site 6

Storage Area 6 – Drilling			**Storage volume (Intermediate)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S(kg)***			***C_{fmax} (g/kg)***
			Max.	***High-end***	***Average***	
111-30-8	Pentanedial/Glutaraldehyde	L	49120	49120	12920	300
11138-66-2	Xanthan gum	S	223400	223400	45300	1000
1305-62-0	Calcium hydroxide (Ca(OH)2)	L	26100	26100	11108	1000
1310-73-2	Sodium hydroxide (Na(OH))	L	2500	2500	2500	500
144-55-8	Carbonic acid, monosodium salt	S	32450	32450	10950	1000
497-19-8	Carbonic acid, disodium salt	S	29125	29125	13050	1000
7447-40-7	Potassium chloride (KCl)	S	197500	197500	197500	1000
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	31600	31600	10725	1000

Table B.35 Hydraulic fracturing chemical concentrations and volumes for Intermediate Storage – Working Site 6

Storage Area 6 – Hydraulic fracturing			**Storage volume (Intermediate)**			**Chemical concentration**
CAS RN	***Chemical***	***State (solid or liquid)***	***V_S (kg)***			***C_{fmax} (g/kg)***
			Max.	***High-end***	***Average***	***Max.***
1310-73-2	Sodium hydroxide (Na(OH))	S	3000	3000	2000	500
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	L	624	624	416	750
64-19-7	Acetic acid	L	20000	20000	8000	600
7647-01-0	Hydrochloric acid	L	50000	50000	13000	320
7647-14-5	Sodium chloride (NaCl)	L	84000	84000	18000	1000
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	S	2200	2200	900	1000
9000-30-0	Guar gum	S	30220	30220	12370	1000
7447-40-7	Potassium chloride (KCl)	S	208000	208000	31000	1000

1.5 References

DoEE 2017, *Environmental exposure conceptualisation for surface to surface water pathways*, report prepared by the Chemical Assessment Section (CAS) of the Department of Environment as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

Appendix C – Model sensitivity analysis

1 Model Sensitivity Analysis

1.1 Runoff model

The paper by Probst et al. (2005) builds on their earlier work (Berenzen et al. 2005). This earlier work examined pesticide (herbicide, fungicide and insecticide) concentrations in 18 small, headwater streams with base flows of approximately 100 to 700 KL per day. The area examined was near Lower Saxony, Germany, and is characterised by undulating or flat (0.5 - 4% slope) intensively farmed agricultural land. The pesticides were automatically sampled and analysed after a rainfall event of 12 mm/day. These sampling sites were within 1 km of the agricultural fields which were ≤ 25 ha and bordering the streams of interest. In addition, measurements were taken for the stream flows during and over the duration of the rainfall event.

The model used several equations (Table C.1) but did not include a correction for heterogeneity. However, it included a factor for foliar interception but assumed that none of this was removed from the plant surface during the rainfall event. A dilution factor (flow of stream x duration of rainfall event) and estimation of application rate of pesticide (in g/ha) was also applied to the %runoff result to predict the concentrations in the streams. The inputs to the model are presented in Table C.1.

Table C.1 Input parameters used by Probst et al. (2005) for the analysis of modelled results

Parameter	Variable*	Source
Runoff in mm/day	R	Lutz (1984) and Maniak (1992)
Precipitation in mm/day	Ψ	Measured
Variable dependent on degradation kinetics of the contaminant and soil	Crsoil_surface	Hornsby et al. (1995)
Organic carbon	O.C.%	Digital soil maps of region
Variable dependent on slope	f1slope	Topographic maps of region
Variable dependent on filtering (see runoff equation in DoEE 2017) buffer default	f2bufferzone	No buffer zones in place form field observations
Parameter dependent on interception	f3foliar_application	Becker et al. (1999)
Application rate	-	Recommended median rates as investigated by Landwirtschaftskammer (2000)
Stream flow	-	Measured

Parameter	Variable*	Source
Duration of rainfall event	-	Measured

For substances known to have been applied approximately three days before the runoff event correlations of r^2 between 0.43 and 0.77 were observed.

1.2 Department of the Environment analysis

A comparison of the values produced by the runoff model with actual measured data from Afyuni *et al.* (1997), showed reasonable agreement. The study involved simulated rainfall of 50.8 mm/hr. This was applied to sites with slopes > 0 - 6%. The average amount of runoff water was 14.1% of the 25.4 mm simulated rainfall. The modelled value for runoff using a hetereogeneity factor of 0.5 and O.C.% of 0.5 - 0.8% for chloriumuron (Koc 110 mL/g but an unknown DT50 in soil) is expected to be between 2.7 - 3.2% of the applied amount and for nicosulfuron (Koc 30 mL/g and DT50 soil of 26 days) between 4.0 - 4.3%. This compared reasonably well with the measured values of applied amount of 1.3% for chloriumuron and 2.8% for nicosulfuron.

A further comparison with Muller et al. (2004) was made for several herbicides including terbuthylazine with less than 24 hours between application and runoff. The study was conducted on very steep slopes (20 and 30%) in New Zealand where the O.C. content of 3.3% is considered low. The percentage runoff volume of water was between 8 - 13% and the Kd value was calculated as approximately 6.4 based on 3.3% O.C. (Koc 194 mL/g). No heterogeneity factor was applied given the small plot sizes (0.5 m^2). Under these quite extreme conditions, the model predicted between 1.1 and 1.8 % of the applied herbicide to runoff, which compared to a measured value of 0.7 - 1.0 %. The model under-predicted the percentage runoff of chemicals with low water solubility due to a high percentage transported in the suspended material phase. It over-predicted for chemicals with very low Koc values likely due to leaching out of the chemical from the runoff active zone before runoff occurred.

1.3 Department of the Environment analysis for atrazine

A further analysis of the values produced by the runoff model was conducted by comparing model results with peak concentrations of atrazine measured in the waterways of the Liverpool Plains. The values used are shown in Table C.2.

Table C.2 Input parameters used for the analysis of modelled results for atrazine

Parameter	Value	Comment
P	100 mm	Likely worst case based on brief survey of Australian weather data
R	20 mm	Based on available evidence especially ANRA (2001) and other sources
Heterogeneity Factor	0.5 based on Dunne and Black (1970)	Based on available evidence
Retention Factor	Zero as determined by Linders et al. (2000)	Bare soil

Parameter	Value	Comment
Environmental transport of suspended pesticides (transport_suspended pesticide)	Zero for pesticides with water solubility ≥ 1 mg/L based on Grover (1989) Water solubility = 33 mg/L (Tomlin 2003)	
Slope	4%, 0.1%	Based on eroded hills and plains (Peirson et al. 1999)
Buffer	1	Default value (no effect)
DT50 soil	Field	41 days (Tomlin 2003) – average value
Koc	39–173	
O.C.	As determined by ANRA (2001) or default of 1% (ibid)	

Modelled concentrations of between 29.8 and 58.6 µg/L were calculated using a 10 ha and 100% treated field at an application rate of 3 kg/ha, with the runoff water entering a 1 500 m^3 stream which is equivalent to a low-flow primary stream (~ 0.03–0.06 m/sec; ~ 0.1–0.2 km/hr) having an approximate dimensions of ~ 2 m wide and ~ 25 cm deep (based on SPDEFTP 2003). This compares with the highest measured peak value of 29 µg/L (Peirson et al. 1999).

1.4 Sensitivity

A sensitivity analysis was performed (Probst et al. 2005) on the parameters (precipitation, runoff volume, half-life, Kd, Koc, %O.C., slope, width of buffer zone and foliar interception). Width of buffer zone and foliar interception were not used in the current consideration as these are not a consideration for current applications in coal seam gas. The DT50 values were varied between 1 - 25 days and the precipitation between 10 - 30 mm/day. The runoff volume was calculated for sandy and loamy bare soils using the methodology of Lutz (1984) and Maniak (1992). There are no details for the variation of % O.C., Koc and slope but this paper asserts that all parameters showed convergence to one demonstrating that they are not sensitive. Based on the equation for slope where slopes over 20% default to one, this is acceptable. Similarly for Kd where the sub-equation is $\frac{1}{1+Kd}$ and Kd can only take positive values, this argument is acceptable when Kd approaches zero.

An illustration of the sensitivity analyses of precipitation and DT50 values is presented below (Figure C.1 and Figure C.2). It was conducted using the formulae dictating these phenomena and extrapolating the reported values of 0.05% *L%runoff* at 10 mm/day rainfall on sandy soil and 0.02% *L%runoff* for a DT50 value of one day.

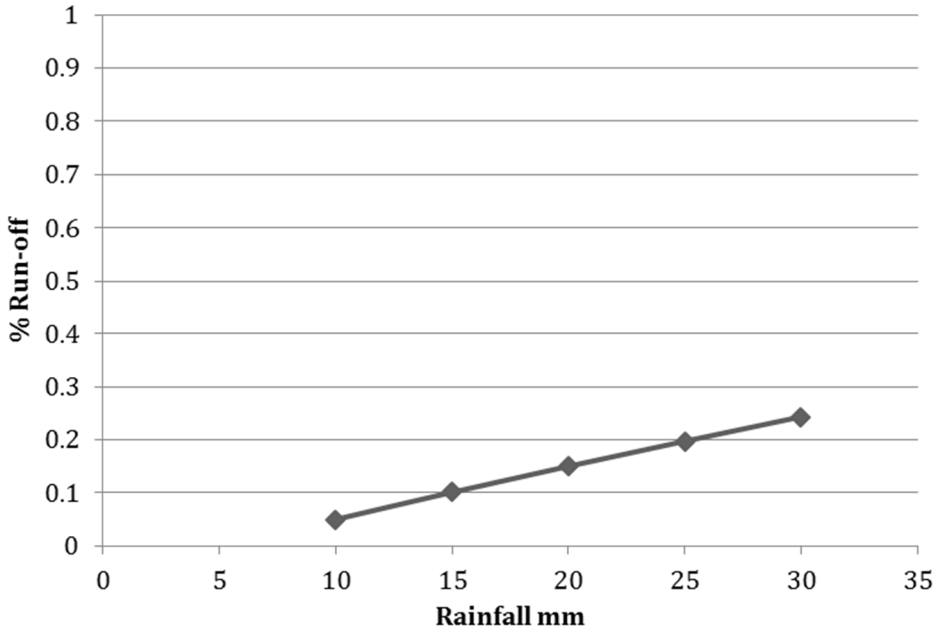

Figure C.1 Sensitivity of the percentage chemical runoff with respect to rainfall

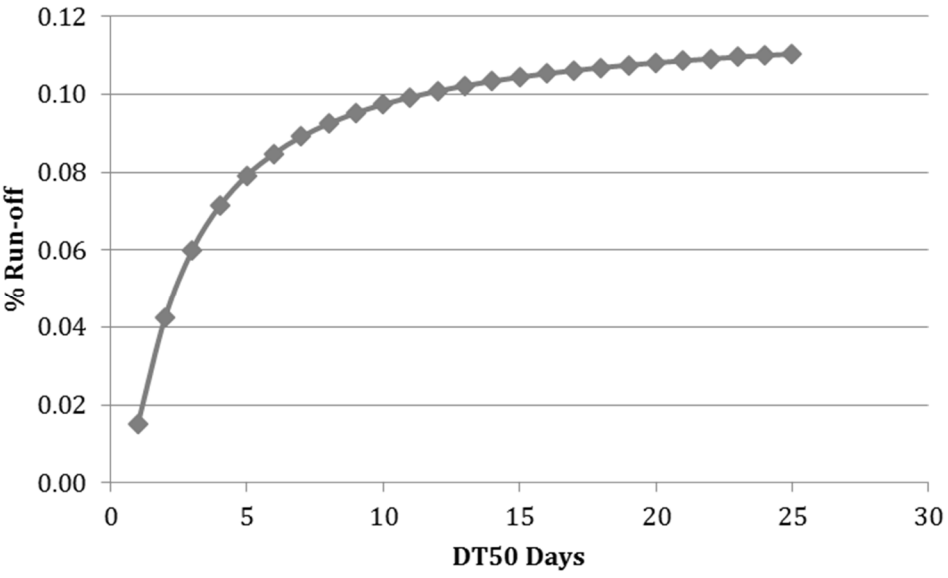

Figure C.2 Sensitivity of the percentage chemical runoff with respect to chemical degradation

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Appendix D – Confidential business information

1 Confidential business information

This Appendix contains confidential business information and has been removed from this public reporting version of the report.

Appendix E – Data tables for calculation of risk quotients

1 Data tables for calculation of risk quotients

This Appendix contains PNECs, PEC, and RQs and is provided separately as downloadable Microsoft Excel spreadsheads.

Appendix F – Regulatory standards for the coal seam gas industry

1 Regulatory standards for the coal seam gas industry

1.1 Regulatory standards for the Queensland coal seam gas industry

Table F.1 Regulatory standards for the Queensland coal seam gas industry

Risk	Legislation / Instrument	Description	How risk is mitigated
Transport risks – e.g. traffic accident, leakage, operator exposure	Australian Dangerous Goods (ADG) Code	Relevant provisions enacted through state legislation *Transport Operations (Road Use Management) Act 1995*	Sets out a range of requirements for workers and organisations including training, routes, goods too dangerous to be transported by road, packaging, incompatibility etc. Also places specific duties on consignors, packers, loaders and drivers to comply with the ADG Code <http://www.ntc.gov.au/heavy-vehicles/safety/australian-dangerous-goods-code/>
	Dangerous Goods Driver Licence	Operator training for avoiding issues and managing emergencies	Ensures drivers have the training to act appropriately <http://www.qld.gov.au/transport/licensing/driver-licensing/applying/dangerous/driver/index.html>
	Dangerous Goods Vehicle Licence	Vehicle operation and technical specification requirements	Ensures vehicles are of appropriate specification, condition and equipped <http://www.qld.gov.au/transport/licensing/driver-licensing/applying/dangerous/vehicle/index.html>
	Dangerous Goods Documents	Records and Emergency Procedure Guide	Enables compliance to be established regarding the transport of the chemicals, as well as assisting in appropriate responses to emergency situations such as spills <https://www.business.qld.gov.au/industry/transport/transporting-

Risk	Legislation / Instrument	Description	How risk is mitigated
			dangerous-goods>
	Work Health and Safety Act 2011	Duty to do everything reasonably practical to keep workers and the general public safe, including adequately addressing risk of chemical exposure	Incumbent upon chemical transport companies to have systems in place to ensure their staff are protected from risks such as crashes and spills. These are in combination with the specific requirements and duties set out in the Dangerous Goods Code. <https://www.legislation.qld.gov.au/LEGISLTN/CURRENT/W/WorkHSA11.pdf> <https://www.worksafe.qld.gov.au/injury-prevention-safety/managing-risks>
	General Environmental Duty	Requirement of the Environmental Protection Act to do everything reasonable and practical to avoid causing harm to the environment.	Incumbent upon chemical transporters to ensure that risks of spilling chemicals (both during transit and transfer operations) are mitigated. These could include only transferring chemicals in contained hardstand areas, having spill response procedures etc.) <https://www.ehp.qld.gov.au/management/planning-guidelines/legislation/general_environmental_duty.html>
	Waste tracking requirements for waste transport (*Environmental Protection Act 1994*)	Requirement of the EP Act to submit waste tracking information to DEHP. The waste tracking system enables the Department to track waste from its source to the place of storage, recycling, treatment or disposal.	Applies to hydraulic fracturing flowback transport – requiring detailed records to demonstrate compliance with the relevant waste management requirements for the particular waste <http://www.ehp.qld.gov.au/waste/pdf/managing-wt-qld-overview.pdf>
Off-tenure product handling risks – e.g. worker contact during bulk mixing and preparation of chemicals; spillage of chemicals; chemical fire	*Environmental Protection Act 1994; Environmental Protection Regulation 2008* – ERA 8	Storing 200 t or more of chemicals triggers Environmentally Relevant Activity 8 – 'Chemical Storage'. In order to legally undertake this activity an environmental authority (EA) under the EP Act is required. This EA contains conditions which are specific to the	Will ensure that environmental risk of the chemical storage and handling activities is adequately controlled. It would be unlikely such a facility would be approved in close proximity to aquatic ecosystems or other environmentally sensitive areas. <https://www.ehp.qld.gov.au/licences-permits/business-industry/index.html> <https://www.legislation.qld.gov.a

Risk	Legislation / Instrument	Description	How risk is mitigated
		operation and require environmental risks to be mitigated. Conditions will likely include bunding and storage requirements (in line with relevant Australian Standards), emergency response procedures, training, monitoring and reporting requirements.	u/LEGISLTN/CURRENT/E/EnvProtR08.pdf>
	Work Health and Safety Act 2011	Duty to do everything reasonably practical to keep workers and the general public safe, including adequately addressing risk of chemical exposure and spills	Incumbent upon chemical storage companies to have systems in place to ensure their staff and the public are protected from risks such as spills and exposure to chemicals. There is also a duty for all staff to follow safety systems and protect themselves and others. These are in combination with the specific requirements of the relevant EA. <https://www.legislation.qld.gov.au/LEGISLTN/CURRENT/W/WorkHSA11.pdf> <https://www.worksafe.qld.gov.au/injury-prevention-safety/managing-risks>
	Sustainable Planning Act 2009	Such a facility would require a development approval assessed against the local planning scheme and relevant state planning instruments. These would include public safety, bushfire risk, proximity of sensitive receptors, proximity of wetlands and many other considerations.	If the facility was to be approved in the proposed location it would have a range of conditions about how the site was to be developed and operated in order to ensure safety and consistency with adjacent land uses. <http://www.dsdip.qld.gov.au/resources/publication/guide-to-spa.pdf>
On-tenure chemical handling (pre-fracture) E.g. worker exposure to chemicals; chemical release to the environment	*Environmental Protection Act 1994* – Resource Activities	The undertaking of activities under the *Petroleum and Gas (Production and Safety) Act 2004* is also classed as an Environmentally Relevant Activity under the EP Act. In	• Restrictions on releasing chemicals to land • A requirement that chemicals must be contained and comply with relevant Australian Standards • Notification of chemical spills • Restriction of activities within

Risk	Legislation / Instrument	Description	How risk is mitigated
while mixing / preparation		order to legally undertake this activity an environmental authority (EA) is required. This EA contains conditions which are specific to the operation and require environmental risks to be mitigated. Due to the higher risks of hydraulic fracturing it is specifically conditioned. A range of more general conditions also apply to the chemical handling associated with hydraulic fracturing.	200 m of HES wetlands ● Restrictions on releasing contaminants to waterways ● Development of contingency procedures for emergencies including risk mitigation measures, remediation measures and investigative procedures ● A site-specific risk assessment of hydraulic fracturing activities to avoid environmental harm and including a list of chemicals to be used and an environmental hazard assessment for these chemicals and human health exposure pathways to operators and the general population ● No use of BTEX or PAH compounds ● No oil or synthetic-based drilling muds ● Monitoring standards and requirements ● Laboratory analysis standards ● requirement to maintain equipment in its proper effective condition. <http://www.ehp.qld.gov.au/management/non-mining/documents/guide-model-conditions-petroleum.pdf> <https://www.ehp.qld.gov.au/management/non-mining/documents/application-requirements-petroleum-guideline.pdf>
	Environmental Protection Act 1994 – EA Conditions	Appropriate protection including infrastructure setbacks and buffers from wetlands, springs, GDE's and watercourses	EA conditions set out approval conditions designe to minimise risks to the environment.
	Petroleum and Gas (Production and Safety) Act 2004 –	A safety management plan (SMP) is required for 'operating plant' which would be interpreted to include	Sets out personal responsibility for safety matters and requires a risk based approach to controls, training, skills and standards. A failure to address safety and

Risk	Legislation / Instrument	Description	How risk is mitigated
	Chapter 9 – Safety management plan	hydraulic fracturing operations, and associated chemical handling. Section 675 of the P and G Act stipulates a detailed list of requirements for SMPs.	health risks associated with chemical handling would be subject to high penalties. Competency requirements for well service workers are also set out through relevant standards under the P and G Act. <http://mines.industry.qld.gov.au/safety-and-health/safeop.htm> <https://www.dnrm.qld.gov.au/__data/assets/pdf_file/0015/240702/competency-std-p-g-well-drilling.pdf>
Chemical Import and manufacturing	*Industrial Chemicals (Notification and Assessment) Act 1989* (Cwlth)	Assessment, inventory, registering and review of industrial chemicals	Aids in the protection of the Australian people and the environment by finding out the risks to occupational health and safety, to public health and to the environment that could be associated with the importation, manufacture or use of industrial chemicals.
Loss of sub-surface containment of fracture fluids risks; e.g. contamination of aquifers; contamination of groundwater resources Handling of chemicals post-hydraulic fracture (on tenure) risks – e.g. soil contamination; seepage into shallow groundwater; worker exposure; exposure in final waste management solution	*Petroleum and Gas (Production and Safety) Act 2004* – well construction and abandonment code	Sets out the minimum requirements in relation to well design, casing, cementing, control equipment, fluids, logging and monitoring.	Ensures that the well will maintain its integrity and not release chemicals into formations other than the target formation. Deals with risks such as casing failure, cementing isolation etc. to ensure that chemicals do not leak out of the well or migrate between formations. <https://www.dnrm.qld.gov.au/__data/assets/pdf_file/0011/119666/code-of-practice-csg-wells-and-bores.pdf>
	Petroleum and Gas (Production and Safety) Regulation 2004 R20, r20A	Requires a notice of intent to hydraulically fracture and a notice of completion of hydraulic fracturing, as well as drilling reports with technical detail around fracturing operations.	Provides government and landholders with an opportunity to comment if any issues are raised with the notice of intent. Also provides specifics to allow rapid responses and ensure compliance. <https://www.legislation.qld.gov.au/LEGISLTN/CURRENT/P/PetroleumR04.pdf>
	Petroleum and Gas (Production and Safety) Act 2004 – Chapter 9 – Safety	A safety management plan is required for 'operating plant' which would be interpreted to include hydraulic fracturing operations.	Sets out personal responsibility for safety matters such as well failure and requires a risk-based approach to controls, training, skills and standards. A failure to address safety and health risks

Risk	Legislation / Instrument	Description	How risk is mitigated
	management plan	Section 675 of the P and G Act stipulates a detailed list of requirements for SMPs.	associated with chemical handling would be subject to high penalties. <http://mines.industry.qld.gov.au/safety-and-health/safeop.htm>
	Environmental Protection Act 1994– Chapter 5, ERA for Resource Activities	The undertaking of activities under the *Petroleum and Gas (Production and Safety) Act 2004* is also classed as an Environmentally Relevant Activity under the EP Act. In order to legally undertake this activity an EA is required. This EA contains conditions which are specific to the operation and require environmental risks to be mitigated. Due to the higher risks of hydraulic fracking it is specifically conditioned. A range of more general conditions also apply to hydraulic fracking including, for example, restrictions on prescribed water contaminants such as those listed in Schedule 9 of the *Environment Protection Regulation 2008.*	• A detailed site-specific risk assessment of hydraulic fracturing including potential environmental and human health risks for water quality and air impacts • Notification of incidents • Restrictions on releasing contaminants to waters • Restrictions on releasing contaminants to land • All waste fluids must be stored in an above ground container (e.g. tank) or in a dam or pond which contains the wetting front • Strict standards for the design, construction and operation of dams, including items such as double lining, leak detection and appropriate design storage allowances <http://www.ehp.qld.gov.au/land/mining/pdf/guide-structures-dams-levees-mining-em634.pdf> • Requirements for annual monitoring of dams and certification and re-certification of medium and high risk dams by suitably qualified registered engineers <https://www.ehp.qld.gov.au/land/mining/pdf/mn-mi-assess-haz-cat-hyd-perf-dams-em635.pdf> • A seepage monitoring program must be developed by a suitably qualified person in order to detect contaminants escaping from ponds or dams*** • Development of contingency procedures for emergencies including risk mitigation measures, remediation measures and investigative procedures • Requirement to site major

Risk	Legislation / Instrument	Description	How risk is mitigated
			ponds outside of environmentally sensitive areas and associated buffers • No use of BTEX or PAH compounds • No oil or synthetic based drilling muds • Any contaminated land is remediated and rehabilitated • Monitoring standards and requirements • Laboratory analysis standards http://www.ehp.qld.gov.au/management/non-mining/documents/guide-model-conditions-petroleum.pdf https://www.legislation.qld.gov.au/legisltn/current/e/envprotr08.pdf
	Environmental Protection Act 1994– Chapter 5, ERA for Resource Activities	EA application requirements for CSG require detailed site-specific information regarding how CSG water and associated wastes will be managed	This site-specific information will need to identify the amount and quality of water that is expected to be produced from both fractured and non-fractured wells. It must then propose: • how the water will be managed • criteria to measure the effectiveness of the management solution • how waste from water management (including flowback water) will be managed This information will then be used to place appropriate requirements on the environmental authority based on how operations will be undertaken <https://www.ehp.qld.gov.au/management/non-mining/documents/application-requirements-petroleum-guideline.pdf> <http://www.ehp.qld.gov.au/management/non-mining/documents/csg-water-measurable-criteria.pdf>.
	Water Act 2000	*Water Reform and Other Legislation*	Under Queensland legislation, petroleum tenure holders may

Risk	Legislation / Instrument	Description	How risk is mitigated
		Amendment Act 2014 will make petroleum tenure holders subject to the water planning and allocation framework for non-associated water	receive rights to extract petroleum resources and to take water as 'associated water'. The exercise of these rights is subject to the petroleum tenure holders complying with underground water obligations under Chapter 3 of the *Water Act 2000*. The *Water Reform and Other Legislation Amendment Act 2014* will amend the *Petroleum and Gas (Production and Safety) Act 2004* to make petroleum tenure holders subject to the water planning and allocation framework for the take of 'non-associated' water. Non-associated water refers to water that is not taken incidentally in extracting the resource, but is taken to use consumptively in a process, such as hydraulic fracturing
	Environmental Protection Act 1994; ERA regulated waste transport.	EA requirement to maintain equipment in its proper and effective condition. EA requirement for daily operation and maintenance of all plant and equipment to be carried out by suitably qualified, competent and experienced person(s)	
	Petroleum and Gas (Production and Safety) Act 2004 – Chapter 9 – Safety management plan	A safety management plan is required for 'operating plant' which would be interpreted to include hydraulic fracturing operations, and associated post-hydraulic fracture waste management. Section 675 of the P and G Act stipulates a detailed list of requirements for SMPs****.	Sets out personal responsibility for safety matters and requires a risk-based approach to controls, training, skills and standards. A failure to address safety and health risks associated with chemical handling would be subject to high penalties. <http://mines.industry.qld.gov.au/safety-and-health/safeop.htm> Competency requirements for well workers are also set out through relevant standards under th P and G Act. <https://www.dnrm.qld.gov.au/__data/assets/pdf_file/0015/240702/competency-std-p-g-well-drilling.pdf>

Risk	Legislation / Instrument	Description	How risk is mitigated
	Coordinator General – Approval Conditions	Assessment of the impacts from hydraulic fracturing chemicals and proposed mitigation measures for hydraulic fracturing chemicals	• A complete inventory of hydraulic fracturing chemicals • Toxicity data for each active ingredient and any mixture of active ingredients • A schedule of stimulation operations • A risk assessment demonstrating that drilling, completions and hydraulic stimulation operations activities will not result in environmental harm to the receiving environment. • Long-term monitoring program of water produced from wells.
	Environment Protection and Biodiversity Conservation Act 1999 (Cwlth) – Approval conditions	Requirements for the development of a Water Monitoring and Management Plan	Conditions designed to protect Mantters of National Environmental Significance. Matters of national environmental significance include 'a water resource, in relation to coal seam gas development and large coal mining development' as well as world and national heritage, wetlands of international importance and listed threatened species and ecological communities The water trigger allows coal and coal seam gas developments that are likely to have a significant impact on water resources to be comprehensively assessed at a national level. As a result of the introduction of the water trigger, the Minister can set appropriate conditions as part of the project approval to ensure that any impacts from these projects on a water resource are acceptable. <https://www.environment.gov.au/water/coal-and-coal-seam-gas>

** More information on the requirement to undertake a detailed stimulation risk assessment is provided below.*

*** More information on fracturing water quality and well monitoring analyte requirements are provided below.*

**** More information on seepage monitoring program requirements are provided below.*
***** More information on the safety management plan requirements are provided below.*

1.1.1 Detailed stimulation risk assessment requirements[32]

The stimulation risk assessment must be carried out for every well prior to stimulation being carried out at that well and address issues at a relevant geospatial scale such that changes to features and attributes are adequately described and must include, but not necessarily be limited to:

1. a process description of the stimulation activity to be applied, including equipment and a comparison to best international practice
2. provide details of where, when and how often stimulation is to be undertaken on the tenures covered by this environmental authority
3. a geological model of the field to be stimulated including geological names, descriptions and depths of the target gas producing formation(s)
4. naturally occurring geological faults
5. seismic history of the region (e.g. earth tremors, earthquakes)
6. proximity of overlying and underlying aquifers
7. description of the depths that aquifers with environmental values occur, both above and below the target gas producing formation
8. identification and proximity of landholder's active groundwater bores in the area where stimulation activities are to be carried out
9. the environmental values of groundwater in the area
10. an assessment of the appropriate limits of reporting for all water quality indicators relevant to stimulation monitoring in order to accurately assess the risks to environmental values of groundwater
11. description of overlying and underlying formations in respect of porosity, permeability, hydraulic conductivity, faulting and fracture propensity
12. consideration of barriers or known direct connections between the target gas producing formation and the overlying and underlying aquifers
13. a description of the well mechanical integrity testing program
14. process control and assessment techniques to be applied for determining extent of stimulation activities (e.g. microseismic measurements, modelling etc.)
15. practices and procedures to ensure that the stimulation activities are designed to be contained within the target gas producing formation
16. groundwater transmissivity, flow rate, hydraulic conductivity and direction(s) of flow
17. a description of the chemical compounds used in stimulation activities (including estimated total mass, estimated composition, chemical abstract service numbers and

[32] Queensland Department of Environment and Heritage Protection, *Environment Protection Act 1994*: Streamlined model conditions for petroleum activities. ESR/2016/1989, ver 2.01, effective: 05 May 16 [https://www.ehp.qld.gov.au/assets/documents/regulation/rs-gl-streamlined-model-conditions-petroleum.pdf].

properties), their mixtures and the resultant compounds that are formed after stimulation

18. a mass balance estimating the concentrations and absolute masses of chemical compounds that will be reacted, returned to the surface or left in the target gas producing formation subsequent to stimulation
19. an environmental hazard assessment of the chemicals used including their mixtures and the resultant chemicals that are formed after stimulation including:
    a. toxicological and ecotoxicological information of chemical compounds used
    b. information on the persistence and bioaccumulation potential of the chemical compounds used
    c. identification of the chemicals of potential concern in stimulation fluids derived from the risk assessment.
20. an environmental hazard assessment of use, formation of, and detection of polycyclic aromatic hydrocarbons in stimulation activities
21. identification and an environmental hazard assessment of using radioactive tracer beads in stimulation activities
22. an environmental hazard assessment of leaving chemical compounds in stimulation fluids in the target gas producing formation for extended periods subsequent to stimulation
23. human health exposure pathways to operators and the regional population
24. risk characterisation of environmental impacts based on the environmental hazard assessment
25. potential impacts to landholder's bores as a result of stimulation activities
26. an assessment of cumulative underground impacts, spatially and temporally of the stimulation activities to be carried out on the tenures covered by this environmental authority
27. potential environmental or health impacts which may result from stimulation activities including but not limited to water quality, air quality (including suppression of dust and other airborne contaminants), noise and vibration.

1.1.2 Hydraulic fracturing water quality and well monitoring analyte requirements[33]

The hydraulic fracturing water quality and well monitoring analyte requirements include:

1. pH
2. electrical conductivity [S/m]
3. turbidity [NTU]

[33] Queensland Department of Environment and Heritage Protection, *Environment Protection Act 1994*: Streamlined model conditions for petroleum activities. ESR/2016/1989, ver 2.01, effective: 05 May 16 [https://www.ehp.qld.gov.au/assets/documents/regulation/rs-gl-streamlined-model-conditions-petroleum.pdf].

4. total dissolved solids [mg/L]
5. temperature [ºC]
6. dissolved oxygen [mg/L]
7. dissolved gases (methane, chlorine, carbon dioxide, hydrogen sulfide) [mg/L]
8. alkalinity (bicarbonate, carbonate, hydroxide and total as CaCO3) [mg/L]
9. sodium adsorption ratio (SAR)
10. anions (bicarbonate, carbonate, hydroxide, chloride, sulphate) [mg/L]
11. ations (aluminium, calcium, magnesium, potassium, sodium) [mg/L]
12. dissolved and total metals and metalloids (including but not necessarily being limited to: aluminium, arsenic, barium, borate (boron), cadmium, total chromium, copper, iron, fluoride, lead, manganese, mercury, nickel, selenium, silver, strontium, tin and zinc) [g/L]
13. total petroleum hydrocarbons [g/L]
14. BTEX (as benzene, toluene, ethylbenzene, ortho-xylene, para- and meta-xylene, and total xylene) [g/L]
15. polycyclic aromatic hydrocarbons (including but not necessarily being limited to: naphthalene, phenanthrene, benzo[a]pyrene) [g/L]
16. sodium hypochlorite [mg/L]
17. sodium hydroxide [mg/L]
18. formaldehyde [mg/L]
19. ethanol [mg/L]
20. gross alpha + gross beta or radionuclides by gamma spectroscopy [Bq/L].

1.1.3 Seepage monitoring program requirements[34]

The seepage monitoring program requirements include:

1. identification of the containment facilities for which seepage will be monitored
2. identification of trigger parameters that are associated with the potential or actual contaminants held in the containment facilities
3. identification of trigger concentration levels that are suitable for early detection of contaminant releases at the containment facilities
4. installation of background seepage monitoring bores where groundwater quality will not have been affected by the petroleum activities authorised under this environmental authority to use as reference sites for determining impacts
5. installation of seepage monitoring bores that:

[34] Queensland Department of Environment and Heritage Protection, *Environment Protection Act 1994*: Streamlined model conditions for petroleum activities. ESR/2016/1989, ver 2.01, effective: 05 May 16 [https://www.ehp.qld.gov.au/assets/documents/regulation/rs-gl-streamlined-model-conditions-petroleum.pdf].safe

   a. are within formations potentially affected by the containment facilities authorised under this environmental authority (i.e. within the potential area of impact)
   b. provide for the early detection of negative impacts prior to reaching groundwater dependent ecosystems, landholder's active groundwater bores, or water supply bores
   c. provide for the early detection of negative impacts prior to reaching migration pathways to other formations (i.e. faults, areas of unconformities known to connect two or more formations).

6. monitoring of groundwater at each background and seepage monitoring bore at least quarterly for the trigger parameters identified in condition (Water 14(b))
7. seepage trigger action response procedures for when trigger parameters and trigger levels identified in conditions (Water 14(b)) and (Water 14(c)) trigger the early detection of seepage, or upon becoming aware of any monitoring results that indicate potential groundwater contamination
8. a rationale detailing the program conceptualisation including assumptions, determinations, monitoring equipment, sampling methods and data analysis
9. provides for annual updates to the program for new containment facilities constructed in each annual return period.

1.1.4 Safety management plan requirements

A safety management plan for an operating plant must include details of each of the following to the extent they are appropriate for the plant:

1. a description of the plant, its location and operations
2. organisational safety policies
3. organisational structure and safety responsibilities
4. each site at the plant for which a site safety manager is required
5. a formal safety assessment consisting of the systematic assessment of risk and a description of the technical and other measures undertaken, or to be undertaken, to control the identified risk
6. if there is proposed, or there is likely to be, interaction with other operating plant or contractors in the same vicinity, or if there are multiple operating plant with different operators on the same petroleum tenure, geothermal tenure or GHG authority:
   a. a description of the proposed or likely interactions, and how they will be managed
   b. an identification of the specific risks that may arise as a result of the proposed or likely interactions, and how the risks will be controlled
   c. an identification of the safety responsibilities of each operator
7. a skills assessment identifying the minimum skills, knowledge, competencies and experience requirements for each person to carry out specific work
8. a training and supervision program containing the mechanism for imparting the skills, knowledge, competencies and experience identified in paragraph 7. and assessing new skills, monitoring performance and ensuring ongoing retention of skill levels

9. safety standards and standard operating and maintenance procedures applied, or to be applied, in each stage of the plant
10. control systems, including, for example, alarm systems, temperature and pressure control systems, and emergency shutdown systems
11. machinery and equipment relating to, or that may affect, the safety of the plant
12. emergency equipment, preparedness and procedures
13. communication systems including, for example, emergency communication systems:
    a. a process for managing change including a process for managing any changes to plant, operating procedures, organisational structure, personnel and the safety management plan
14. the mechanisms for implementing, monitoring and reviewing and auditing safety policies and safety management plans
15. key performance indicators to be used to monitor compliance with the plan and this Act
16. mechanisms for:
    a. recording, investigating and reviewing incidents at the plant
    b. implementing recommendations from an investigation or review of an incident at the plant
17. record management, including, for example, all relevant approvals, certificates of compliance and other documents required under this Act
18. to the extent that, because of the Work Health and Safety Act 2011, schedule 1, part 2, division 1, that Act does not apply to a place or installation at the plant, details, including codes and standards adopted, addressing all relevant requirements under that Act that would, other than for that section, apply
19. if the operating plant is, under the NOHSC standard, a major hazard facility – each matter not mentioned in paragraphs (b) to (r) that is provided for under chapters 6 to 10 of that standard.

1.2 Regulatory standards for the New South Wales coal seam gas industry

Table F.2 Regulatory standards for the New South Wales coal seam gas industry

Risk	Legislation / Instrument	Description	How risk is mitigated
Transport risks – e.g. traffic accident, leakage, operator exposure	Australian Dangerous Goods code	Relevant provisions enacted through state legislation *Dangerous Goods (Road and Rail Transport) Act 2008* and *Dangerous Goods (Road and Rail Transport) regulation 2014*	Hazardous materials are substances falling within the classification of the Australian Code for *Transportation of Dangerous Goods by Road and Rail (Dangerous Goods Code)* The EPA regulates the on-road transport of dangerous goods while WorkCover regulates

Risk	Legislation / Instrument	Description	How risk is mitigated
			activities prior to transport, including correct classification, packaging and labelling. These are effectively the same as the Queensland regime as they are both based on national model legislation. <http://www.legislation.nsw.gov.au/sessionalview/sessional/sr/2014-398.pdf>
	Dangerous Goods Driver Licence	Operator training for avoiding issues and managing emergencies	Ensures drivers have the training to act appropriately
	Dangerous Goods Vehicle Licence	Vehicle operation and technical specification requirements	Ensures vehicles are of appropriate specification, condition and equipped
	Dangerous Goods Documents	Records and Emergency Procedure Guide	Enable compliance to be established regarding the transport of the chemicals, as well as assisting in appropriate responses to emergency situations such as spills
	Work Health and Safety Act 2011	Duty to for officers to exercise due diligence to ensure safety of employees and duty of workers to ensure safety of themselves and other persons and comply with instructions	Incumbent upon chemical transport companies to have systems in place to ensure their staff are protected from risks such as crashes and spills. These are in combination with the specific requirements set out in the Dangerous Goods Code. <http://www.legislation.nsw.gov.au/maintop/view/inforce/act+10+2011+cd+0+N>
	Environmental offences	The *Protection of the Environment Operations Act 1997* provides offences for wilfully or negligently causing harm to the environment.	Incumbent upon chemical transporters to ensure that risks of spilling chemicals (both during transit and transfer operations) are mitigated. These could include only transferring chemicals in contained hardstand areas, having spill response procedures etc. The Environment Protection Authority (EPA) has the power to inspect and prosecute companies for environmental and health breaches. <http://www.epa.nsw.gov.au/legislation/aboutpoeo.htm#P90_6221>

Risk	Legislation / Instrument	Description	How risk is mitigated
	Waste tracking requirements for waste transport	The *Protection of the Environment Operations (Waste) Regulation 2005* implements requirements to track and record the transportation of high environmental risk wastes.	Would likely apply to frack flowback transport – requiring detailed records to demonstrate compliance with the relevant waste management requirements for the particular waste <http://www.legislation.nsw.gov.au/inforcepdf/2005-497.pdf?id=15937bef-eef8-c8ed-d2c1-dd4c148cc79c>
Off-tenure product handling risks – e.g. worker contact during bulk mixing and preparation of chemicals; spillage of chemicals; chemical fire	Environmental Protection Licence – Chemical Storage	Storing 5 000 kL or more of chemicals triggers a requirement for an Environment Protection Licence (EPL). EPLs contains conditions which are specific to the operation and require environmental risks to be mitigated.	Will ensure that environmental risk of the chemical storage and handling activities is adequately controlled. It would be unlikely such a facility would be approved in close proximity to aquatic ecosystems or other environmentally sensitive areas. <http://www.legislation.nsw.gov.au/#/view/regulation/2009/211/full>
	Work Health and Safety Act 2011	Duty for officers to exercise due diligence to ensure safety of employees and duty of workers to ensure safety of themselves and other persons and comply with instructions	Incumbent upon companies handling chemicals to have systems in place to ensure their staff are protected from risks such as exposure and spills. These are in combination with the specific requirements set out in the PEL if over the 5 000 kL threshold. <http://www.legislation.nsw.gov.au/maintop/view/inforce/act+10+2011+cd+0+N>
	Environmental Planning and Assessment Act 1979	Such a facility would require a development application be submitted to Council and assessed against the planning scheme and relevant state instruments. May also go to joint regional planning panel for regional development.	If the facility was to be approved in the proposed location it would be likely to have a range of conditions, about how the site was to be developed and operated in order to ensure safety and consistency with adjacent land uses. <http://www.legislation.nsw.gov.au/maintop/view/inforce/act+203+1979+cd+0+N>
On-tenure chemical handling (pre-fracture) E.g. worker exposure to chemicals; chemical release to the environment	*Protection of the Environment Operations Act 1997*	The undertaking of coal seam gas exploration and production activities triggers a requirement for an Environment Protection Licence	Requires compliance with a range of conditions built around mitigating impacts associated with discharges to land, air and water. Requires the preparation of pollution incident response management plans and or pollution reduction programs for non-compliance with EPL

Risk	Legislation / Instrument	Description	How risk is mitigated
while mixing / preparation			conditions. These conditions have requirements relating to contingency management and chemical storage standards etc. No 'model conditions' for CSG EPLs are currently available, however examples can be obtained from various recent approvals. <http://www.legislation.nsw.gov.au/sessionalview/sessional/sr/2014-852.pdf>
	Petroleum (Onshore) Act 1991 and *Work Health and Safety Act 2011*	The Office of Coal Seam Gas has responsibility for implementation of safety requirements for the CSG industry, including those around chemical handling and storage. Both pieces of legislation apply.	It is incumbent upon companies handling chemicals to have systems in place to ensure their staff are protected from risks such as exposure and spills. <http://www.epa.nsw.gov.au/resources/licensing/150118-petroleum-regulatory-controls.pdf> <http://www5.austlii.edu.au/au/legis/nsw/consol_act/whasa2011218> <http://www.legislation.nsw.gov.au/#/view/act/1991/84/full>
	Code of Practice for Fracture Stimulation	The Code of Practice for Fracture Stimulation has been approved by the Minister for Resources and Energy and is mandatory for CSG operators	The Code of Practice for CSG fracking provides that chemical use should be minimised and prevents the use of BTEX chemicals. It also requires a fracture stimulation management plan, which outlines: • the volumes and concentrations of those chemicals • potential risks to human health arising from exposure to those chemicals • the risk, likelihood and consequence of surface spills of these chemicals • how those chemicals will be stored and managed. The code also provides for the development of an Emergency Plan dealing with matters such as evacuation procedures, medical treatment and assistance and training requirements. Further, the code provides for the mandatory development of an Environmental Incident Response Plan dealing with matters

Risk	Legislation / Instrument	Description	How risk is mitigated
			including chemical spills and other pollution incidents including: • details of the pre-emptive action to be taken to minimise or prevent any risk of harm to human health or the environment arising out of the activity • an inventory of potential pollutants on the premises or used in carrying out the activity, • the maximum quantity of any pollutant that is likely to be stored or held at the location of the fracture stimulation activity • a description of the safety equipment or other devices that are used to minimise the risks to human health or the environment and to contain or control a pollution incident • details of the mechanisms for providing early warnings and regular updates to the owners and occupiers of premises in the vicinity of the fracture stimulation activity • the arrangements for minimising the risk of harm to any persons who are present where the fracture stimulation activity is being carried out. <http://www.resourcesandenergy.nsw.gov.au/__data/assets/pdf_file/0018/516114/Code-of-Practice-for-Coal-Seam-Gas-Fracture-Stimulation.pdf>
Loss of sub-surface containment of fracture fluids risks; e.g. contamination of aquifers; contamination of groundwater resources	Well Integrity Code	Sets out the mandatory minimum requirements in relation to well construction to ensure integrity.	Requires risk management planning to be applied to well operations in the context of the *Work Health and Safety Act 2011* and further requires a Safety Management Plan to be developed for each stage of well operations. The code details reporting requirements including a record of all work undertaken on a well*. Cementing reports are also required in order to demonstrate isolation. Extensive requirements to ensure

Risk	Legislation / Instrument	Description	How risk is mitigated
			that no loss of containment are stipulated in relation to the following: • well design (including casing setting depths accounting for aquifers and production zone locations) • casing (e.g. designed to withstand loads and pressures and meet API standards) • cementing (including cementing from shoe to surface and verification of zonal isolation) • well heads (to API standards) • drilling fluids (including no oil-based muds, records of each chemical used and managed in accordance with MSDS requirements) • evaluation (well downhole survey carried out) • ongoing appropriate monitoring and maintenance • suspension and abandonment (including extensive requirements to ensure safety and integrity of the well into the foreseeable future). <http://www.resourcesandenergy.nsw.gov.au/__data/assets/pdf_file/0018/516114/Code-of-Practice-for-Coal-Seam-Gas-Fracture-Stimulation.pdf>
	Code of Practice for Fracture Stimulation	The Code of Practice for Fracture Stimulation has been approved by the Minister for Resources and Energy and is mandatory for CSG operators	Contains extensive detailed requirements and implements a risk-based approach to ensuring safety and environmental outcomes in relation to hydraulic fracturing activities. Requires a fracture stimulation management plan* be in place prior to fracturing including in relation to fracture stimulation design, assessment of risks, protection of water resources and monitoring requirements. Further, the code requires an Environmental Emergency Response Plan which deals specifically with loss of well integrity.

Risk	Legislation / Instrument	Description	How risk is mitigated
			A completion report must be submitted following fracturing events which demonstrates that no environmental harm has been caused. <http://www.resourcesandenergy.nsw.gov.au/__data/assets/pdf_file/0018/516114/Code-of-Practice-for-Coal-Seam-Gas-Fracture-Stimulation.pdf>
	Protection of the Environment Operations Act 1997	The undertaking of CSG exploration and production activities triggers a requirement for an Environment Protection Licence	Requires the preparation of pollution incident response management plans and compliance with a range of conditions. These conditions have requirements relating to the undertaking of fracture stimulation activities. No 'model conditions' for CSG EPLs are currently available, however examples can be obtained from various recent approvals. <http://www.legislation.nsw.gov.au/sessionalview/sessional/sr/2014-852.pdf>
	Strategic Regional Land Use Policy	An Agricultural Impact Statement (AIS) is now required for various minerals and petroleum (incl. CSG) activities at the exploration and development application stages	A comprehensive Agricultural Impact Statement must be provided by the applicant at both the exploration stage (where there is a requirement for a Review of Environmental Factors) and at the development application stage. <http://www.resourcesandenergy.nsw.gov.au/miners-and-explorers/rules-and-forms/pgf/guidelines/agricultural-impact-statements>
	Water Management Act 2000	A Water Access License is required to take water in the course of undertaking a mining activity.	Determines requirements for taking groundwater, whether for consumption or incidentally, unless an exemption applies. Any new mining and petroleum exploration activities that take more than three megalitres per year from groundwater sources will need to hold a WAL.
	Protection of the Environment Operations Act 1997	The undertaking of CSG exploration and production activities triggers a requirement for an Environment Protection Licence	Requires the preparation of pollution incident response management plans and compliance with a range of conditions. These conditions have requirements relating to the

Risk	Legislation / Instrument	Description	How risk is mitigated
			undertaking of fracture stimulation activities. Flowback water is defined as a liquid waste which must be managed, stored, transported and disposed of in a way that protects the environment and in accordance with the EPL condition requirements. The EPA requires that flowback water must be appropriately stored and transported to a facility that is licensed by the EPA to take that type of waste. All CSG facilities must also keep detailed records of their liquid waste. No 'model conditions' for CSG EPLs are currently available, however examples can be obtained from various recent approvals. <http://www.legislation.nsw.gov.au/sessionalview/sessional/sr/2014-852.pdf> <http://www.epa.nsw.gov.au/resources/licensing/150007csgflowbackwater.pdf>
Handling of chemicals/flowback post-fracture (on tenure) risks – e.g. soil contamination; seepage into shallow groundwater; worker exposure; exposure in final waste management solution	Code of Practice for Fracture Stimulation	The Code of Practice for Fracture Stimulation has been approved by the Minister for Resources and Energy and is mandatory for CSG operators	Contains extensive detailed requirements and implements a risk-based approach to ensuring safety and environmental outcomes in relation to hydraulic fracturing activities. Requires a fracture stimulation management plan be in place prior to fracturing including in relation to fracture stimulation design, assessment of risks, protection of water resources and monitoring requirements. It is specifically required to detail the management storage and disposal of flowback water. Further, the code requires an Environmental Emergency Response Plan which deals specifically with spills. A completion report must be submitted following fracturing events which demonstrates that no environmental harm has been caused. <http://www.resourcesandenergy.nsw.gov.au/__data/assets/pdf_file

Risk	Legislation / Instrument	Description	How risk is mitigated
			/0018/516114/Code-of-Practice-for-Coal-Seam-Gas-Fracture-Stimulation.pdf>
	Petroleum (Onshore) Act 1991 and Work Health and Safety Act 2011	The Office of Coal Seam Gas has responsibility for implementation of safety requirements for the CSG industry, including those around chemical handling and storage. Both pieces of legislation apply.	It is incumbent upon companies handling chemicals to have systems in place to ensure their staff are protected from risks such as exposure and spills. <http://www.epa.nsw.gov.au/resources/licensing/150118-petroleum-regulatory-controls.pdf> <http://www5.austlii.edu.au/au/legis/nsw/consol_act/whasa2011218/>. <http://www.legislation.nsw.gov.au/#/view/act/1991/84/full>

** More information on good industry practice well records is provided below.*
*** More information on requirements for fracture stimulation management plans is provided below.*

1.2.1 Good industry practice for well records

Good industry practice for well records include:

1. engineering design basis
2. kick tolerance/well control design assumptions
3. BOP pressure testing requirements, and actual test records
4. laboratory test results for cement slurries
5. casing tallies for all casing strings run (including lengths, weights, grades, inside diameter, outside diameter, setting depth)
6. cementing records for each casing string in each well
7. casing pressure test reports
8. leak-off test and / or formation integrity test reports
9. wireline logs
10. core description reports
11. downhole installation records/schematic
12. records of chemicals used downhole, including any chemicals used in drilling fluid, treatment and workover or other well procedures (name, type CAS number and volume of each chemical used should be recorded)
13. records of drilling and cementing, including any problems encountered during the drilling
14. risk assessments
15. well drilling and completion programs including casing running and cementing procedures

16. daily rig reports
17. daily geological reports, if relevant
18. service company reports.

1.2.2 Requirements for fracture stimulation management plans

The requirements for fracture stimulation management plans in New South Wales are provided below:

1. fracture stimulation activities must not be conducted except in accordance with a FSMP approved by the department
2. the FSMP must describe the nature, location, scale, timing, duration, hours of operation and other relevant features of the fracture stimulation activity
3. the FSMP must demonstrate that all risks to the environment, existing land uses, the community and workforce, as a result of the fracture stimulation activity, are managed through an effective risk management process that includes identification of hazards, assessment of risks, implementation of control measures and monitoring of the integrity and effectiveness of the control measures
4. the FSMP must identify how the titleholder will address and comply with the requirements of this Code
5. the FSMP must be reviewed and as necessary revised by the titleholder:
    a. before making a significant change to the design or operation of the fracture stimulation activity
    b. if the sensitivity of potentially affected environmental, land use or community features significantly increases
    c. in the event that monitoring indicates that the consequences of the fracture stimulation activity exceed those identified in the FSMP, or that a risk control measure does not adequately control the risk Fracture Stimulation Activities
6. the detail provided in the FSMP must be appropriate to the nature, scale, intensity and potential impacts of the proposed fracture stimulation activity
7. the FSMP is a public document and may be published by the department on its website or by other means. Commercially sensitive or personal information should not be included within a FSMP unless specifically required by this Code.

The design of the fracture stimulation activity must be described in the FSMP. This description must incorporate the following:

1. characterisation of geological formations, including the identification of rock types and conditions, aquifers and hydrocarbon-bearing zones
2. definition of distances to these aquifers from the target coal beds
3. identification of the characteristics of intervening strata, including porosity/permeability and the extent of natural fracturing
4. determination of geological stress fields and areas of faulting
5. determination of maximum pressures to be used for fracture stimulation, based on the characteristics of the surrounding geology

6. modelling of the likely fracture propagation field, including extent and orientation
7. discussion of any potential for the fracture propagation field to exceed that modelled in paragraph 6.

The FSMP must include a risk assessment complying with AS/NZS ISO 31000:2009 Risk management - Principles and Guidelines. It must also:

1. identify risks associated with the fracture stimulation activity, the likelihood of each risk and the consequence of each risk
2. define appropriate management controls to ensure identified risks are constrained to acceptable levels
3. at a minimum, the risk assessment must address risks associated with:
    a. workplace health and safety (see heading 5 of this Code)
    b. public safety (see heading 5 of this Code)
    c. chemical use (see heading 6 of this Code)
    d. impacts on water resources (see headings 7 and 8 of this Code)
    e. land contamination
    f. air pollution
    g. noise and vibration
    h. waste management (e.g. flowback water as per heading 8 of this Code)
    i. loss of well integrity
    j. induced seismicity
    k. induced subsidence or other induced ground movements
    l. conflicts with existing land uses.

1.2.3 Water resources

The FSMP must identify the location, extent, pre-existing water quality and use of water sources which have the potential to be impacted by the fracture stimulation activity. It must also:

1. identify sources of fracture stimulation injection water, the estimated quality and volume to be injected and any licensing/approval requirements under the *Water Management Act 2000* or *Water Act 1912*
2. include a qualitative risk assessment for risks associated with the fracture stimulation activity, including:
    a. cross-contamination between coal bed waters and shallower water sources
    b. changes to groundwater pressure and levels
    c. changes to surface water levels
    d. changes to water quality characteristics
3. if the risk of establishing a connection between the target coal bed and other water sources as a result of the fracture stimulation activity is assessed to be moderate or higher, then a fate and transport model study must be undertaken to quantify the

impacts on water sources and the likelihood of any changes to the beneficial use category applicable to any affected aquifer

4. if there is a moderate or greater risk of significant changes to pressure or levels as referred to in paragraph 3.b or 3.c, the impacts on all affected aquifers must be quantitatively assessed
5. describe consultation undertaken with the NSW Office of Water in developing the water resources component of the risk assessment.

The FSMP must describe any monitoring arrangements, including monitoring before, during and after the fracture stimulation activity. This includes requirements for:

1. the titleholder to carry out sufficient monitoring to establish that significant risks have been:
    a. identified
    b. quantified
    c. avoided, or appropriately managed so that residual risks are within acceptable limits before, during and after the fracture stimulation activity
2. monitoring of overlying water sources to be undertaken over an area sufficient to encompass the predicted fracture length plus a sufficient margin to provide for any uncertainty
3. prior to fracture stimulation, monitoring to be undertaken to characterise water source level, pressure and quality. This monitoring should include existing wells and water bores at a minimum
4. during fracture stimulation, monitoring to be undertaken to:
    a. record key parameters such as bottom hole pressure and surface injection pressure
    b. establish the volume, composition, viscosity and pumping rate of fracture fluids and proppants
5. post-stimulation, monitoring to be undertaken to ensure that induced inter-aquifer connectivity has been prevented by:
    a. determining the volume and quality of flowback and produced water
    b. quantifying any changes in surrounding water sources
    c. pressure testing of casing to verify that the integrity of the well and well equipment has been maintained.

Appendix G – Compiled qualitative risk assessments of 54 chemicals

1 Hydrogen peroxide

1.1 Background

Hydrogen peroxide is a naturally occurring chemical, and is produced by almost all cells as a part of normal metabolic processes (OECD 1999). It is also commercially available as aqueous solutions varying in concentration from 2 to 90% w/w, and is used as an oxidant for dyeing hair, as a topical disinfectant, in pulp bleaching, in textile bleaching, in chemical processing, and in wastewater treatment (EC CAB 2000; EC 2003). Hydrogen peroxide is used in the coal seam gas industry as a 'breaker' to chemically degrade the gel in hydraulic fracturing fluids in order to reduce the viscosity back to that of water (DotE 2014). According to information from the Queensland Government, its use within the Australian coal seam gas industry is for gel management (DoEHP QG 2015).

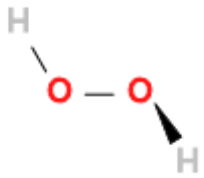
Hydrogen peroxide is formed and transformed by natural processes in each compartment of the environment through biotic and abiotic reactions, with irradiation of water producing 2 to 12 µg per hour per litre in freshwater ecosystems (Wetzel 2001; EC CAB 2000). The mean measured background concentration of hydrogen peroxide in air and lake water has been reported as 0.14 to 1.4 µg/m^3 (0.1 to 1 ppb) and 1 to 30 µg/L, respectively. The peak concentration of hydrogen peroxide in air and lake water has been reported as 10 µg/m^3 (7 ppb) and >100 µg/L, respectively (EC 2003).

Hydrogen peroxide is a reactive colourless liquid at room temperature (ATSDR 2002). It is a strongly oxidising chemical that undergoes a variety of rapid redox reactions in aqueous solution that result in its decomposition. An important route of degradation of hydrogen peroxide in surface waters is the highly exothermic disproportionation of hydrogen peroxide to water and molecular oxygen (dioxygen). This reaction proceeds by both abiotic and biotic pathways in environmental waters. The abiotic disproportionation of hydrogen peroxide is catalysed by a variety of environmental species, especially transition metal ions. The disproportionation of hydrogen peroxide is also catalysed by catalase enzymes, which are ubiquitous in the cells of aerobic life forms (EC 2003).

The reactive nature of hydrogen peroxide means that it can cause oxidative stress in exposed organisms. In addition, its reactions with water constituents can increase water temperatures abruptly (ATSDR 2002) and potentially burn any organisms which come into contact before it breaks down into water and oxygen. However, the short lifetime of hydrogen peroxide in soil and water and further normal biogeochemical regulation mechanisms are expected to limit the potential for the chemical to cause any such effects in the environment.

1.2 Chemical name and identification

CAS Name	**Hydrogen peroxide (H_2O_2)**
CAS RN	7722-84-1

CAS Name	**Hydrogen peroxide (H_2O_2)**
AICS name	Hydrogen peroxide (H_2O_2)
Synonyms	Hydrogen peroxide Dihydrogen dioxide
Structural formula	
Molecular formula	H_2O_2
Molecular weight	34.01 g/mol
SMILES	OO

1.3 Physico-chemical properties

Pure hydrogen peroxide is stable at normal temperature and pressure. Commercial solutions must be stabilised with additives to prevent possibly violent decomposition due to catalytic impurities or elevated temperatures and pressures. Stability is at a maximum at pH 3.5 to 4.5. Hydrogen peroxide is not flammable, however, it presents a fire hazard because as a strong oxidizer it can enhance the combustion of other substances (EC 2003):

Property	
Physical form	Colourless, clear syrupy liquid and highly volatile under ambient conditions (EC 2003)
Melting point	-0.41°C (Hess 1999)
Boiling point	150–152°C (EC 2003)
Density (relative to water)	1.4425 g/cm^3 at 25°C (EC 2003)
Water solubility	Miscible in all proportions (Hess 1999)
pK_a	11.62 at 25°C (EC 2003)
Log K_{ow}	Not applicable
Vapour pressure	300 Pa at 25°C (EC 2003)

1.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for hydrogen peroxide:

Pre-assessment profile	
Montreal	No
SGG	No

Pre-assessment profile	
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

1.5 Environmental fate summary

1.5.1 Dissolution, speciation and partitioning

Hydrogen peroxide is stable under ambient conditions as a pure liquid, however, aqueous solutions are unstable with respect to spontaneous decomposition to oxygen and water (Hess 1999; Cotton and Wilkinson 1988). Under environmental conditions, hydrogen peroxide is expected to decompose rapidly. Therefore, partitioning of the chemical beyond the compartment of release is not expected.

The decomposition of hydrogen peroxide in aqueous solution is a disproportionation reaction (Equation G1), which is catalysed by transition metal ions, dust, and alkali (EC 2003):

$$2H_2O_2 \rightarrow H_2O + O_2 \qquad \text{[Equation G1]}$$

Hydrogen peroxide is a strong oxidant in acid and basic solution. It can also react as a modest reductant, although only towards powerful oxidants such as Cl_2. The rate of oxidation by hydrogen peroxide is slow in acid solution and fast in basic solution (Cotton and Wilkinson 1988). Hydrogen peroxide also undergoes substitution chemistry.

1.5.2 Persistence

Hydrogen peroxide is biologically degradable by aerobic organisms. Degradation of the chemical is therefore highly dependent on biological composition, as well as the presence of metal catalysts (EC 2003). The half-life of hydrogen peroxide in soil without microbiological activity and few minerals has been reported as 15 hours as compared with only several minutes in soil with 10^8 to 10^9 cells/g total solids and which also contained iron and manganese at catalysts. The half-life for hydrogen peroxide in ground water was in the range 7 to 70 minutes (ECETOC 1993).

In surface waters, hydrogen peroxide undergoes abiotic degradation through disproportionation and redox reactions. It is also degraded by algae and microorganisms, and the lifetime of H_2O_2 in natural surface waters is therefore strongly influenced by the biological composition of the water body (ECETOC 1993). The half-life in water depends on the exposure conditions, but a short half-life has been reported at pH 7 (US EPA 2007).

The degradation half-life for hydrogen peroxide in the atmosphere has been variously estimated as in the range 10 to 20 hours for the troposphere (ECETOC 1993) to an average of 24 hours (EC 2003). Based on the above experimental values hydrogen peroxide is not considered persistent in the environment.

1.5.3 Bioaccumulation

There are no experimental results on bioaccumulation available, however, the potential for hydrogen peroxide to bioaccumulate is mitigated by enzymes such as catalase which naturally regulate the levels of hydrogen peroxide in aerobic organisms. Therefore, no bioaccumulation is expected.

1.5.4 Transport

Hydrogen peroxide is a naturally occurring, globally distributed chemical. The chemical rapidly degrades in all environmental compartments as a result of biotic and abiotic reactions. No significant potential for long-range transport is expected.

1.6 Environmental effects summary

1.6.1 Critical environmental effects

1.6.1.1 Acute toxicity endpoints for aquatic organisms

The median lethal concentration (LC50) and median effective concentration (EC50) values for model organisms across three trophic levels were used to characterise the acute effects of this chemical (EC 2003):

Taxon	Endpoint	Method
Fish	96 h LC50 = 16.4–37.4 mg/L	Experimental Pimephales promelas
Invertebrates	96 h EC50 = 2.3–17.7 mg/L	Experimental Daphnia spp.
Algae	EC50 = 1.6–43 mg/L	Experimental Anabaena A4

The effects of hydrogen peroxide on micro-organisms have been assessed. The EC50 of 466 mg/L for inhibition of microbial respiration in sludge micro-organisms indicates hydrogen peroxide is non-inhibitory to microbial respiration (EC 2003).

1.6.1.2 Chronic toxicity endpoints for aquatic organisms

The following No-Observed-Effect-Concentration (NOEC) values for model organisms from two major aquatic trophic levels were used to characterise the chronic effects of this chemical (EC 2003):

Taxon	Endpoint	Method
Fish	Not available	-
Invertebrates	56 d NOEC = 2 mg/L	Experimental Zebra mussels (species not specified)
Algae	72 h NOEC = 0.1–0.63 mg/L	Experimental *Chlorella vulgaris*

Based on the above toxicity data, hydrogen peroxide is not categorised as toxic to aquatic life according to domestic toxicity criteria.

1.7 Categorisation and other characteristics of concern

1.7.1 PBT categorisation

The chemical is not a PBT substance according to domestic environmental hazard criteria.

1.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for this chemical.

1.8 Screening assessment

1.8.1 Assessment

Hydrogen peroxide is a naturally occurring and ubiquitous chemical in the environment. It is naturally produced and degraded through a range of biotic and abiotic reactions. Under typical environmental conditions, the chemical is expected to degrade rapidly in soil and water and does not persist in the environment. The chemical also does not bioaccumulate. Hydrogen peroxide has some moderate acute toxicity to aquatic organisms, but all aerobic aquatic organisms are naturally adapted to fluctuating background concentrations of hydrogen peroxide in natural waters.

Release of large volumes of hydrogen peroxide directly into the environment may create physico-chemical stressors. For example, its reactions with water constituents can increase water temperatures abruptly (ATSDR 2002) and potentially burn any organisms which come into contact before it breaks down into water and oxygen. Release of hydrogen peroxide can also affect the oxidation state and speciation of metal ions in the environment. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate fluctuations in the concentrations of hydrogen peroxide in aquatic ecosystems. The chemical is highly reactive in soil and any direct releases to soil are expected to result in spontaneous and rapid degradation of hydrogen peroxide to water and dioxygen. Hence, indirect emissions of H_2O_2 to surface waters as a result of releases of the chemical to the soil compartment through spills or use in coal seam gas extraction are not expected to occur.

1.9 Outcome

A Tier 1 assessment of the environmental risks from the use of hydrogen peroxide is not required.

1.10 References

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2 Sodium acetate

2.1 Background

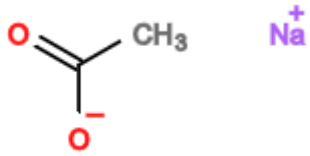
Acetic acid, sodium salt (sodium acetate) has a wide range of industrial and domestic uses, including as a food additive, paint additive, and for photography (Nordic Council of Ministers 2014). The products in which sodium acetate occurs and its function within the domestic coal seam gas industry were not specified in survey information supplied for this report. However, it is noted that sodium acetate is a salt of acetic acid, and acetic acid is widely used in the coal seam gas industry as a pH adjuster and for iron control (Stringfellow et al. 2014).

Dissolution of sodium acetate will result in hydrolysis of acetate to form acetic acid (a weak carboxylic acid), depending on environmental conditions. At neutral pH, hydrolysis will be limited and acetic acid will exist predominately in its conjugate base (acetate ion) form. Acetate is ubiquitous in natural water and acts as a key nutrient, supplying energy to heterotrophic algae under aerobic conditions (Wetzel 2001). Acetate is also formed by anaerobic bacteria through natural fermentation processes as a source of energy (Levin 2009; Wetzel 2001). The chemical can also be formed by hydrolysis and through photolysis of naturally occurring substances. Concentrations of acetate generally remain low in natural water bodies as its input rate is roughly balanced by the rate of bacterial uptake (Wetzel 2001).

Sodium ions will also be released upon dissolution of sodium acetate. However, sodium ions are similarly naturally ubiquitous in the environment, and have low toxicity. The information presented in this assessment is generally for acetic acid, reflecting levels of inherent concern and corresponding data availability.

Release of large volumes of sodium acetate (or acetic acid) to natural waterways may disturb the health of aquatic ecosystems through direct and indirect physical and chemical effects. For example, at very high concentrations, these chemicals have the potential to modify the pH beyond normal ranges (ANZECC and ARMCANZ 2000). Further, rapid biodegradation of large quantities of these chemicals in natural water bodies may decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life (Stringfellow et al. 2014). However, numerous natural biogeochemical mechanisms exist which tend to limit fluctuations in nutrient levels, which occur frequently in healthy aquatic ecosystems.

2.2 Chemical name and identification

CAS Name	**Acetic acid, sodium salt**
CAS RN	127-09-3
AICS name	Acetic acid, sodium salt
Synonyms	Sodium acetate
Structural formula	

CAS Name	Acetic acid, sodium salt
Molecular formula	$C_2H_3NaO_2$
Molecular weight	82.03 g/mol
SMILES	C(C)(=O)[O-].[Na+]

2.3 Physico-chemical properties

Property	
Physical form	Solid
Melting point	324.0°C (LMC 2014)
Boiling point	Not available
Water solubility	1190 g/L (Weast 1976)
pK_a	4.76 (Acetic acid LMC 2014)
Log K_{ow}	-0.17 (Acetic acid LMC 2014)
Vapour pressure	Not available

2.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for sodium acetate or acetic acid:

Preassessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

2.5 Environmental fate summary

2.5.1 Dissolution, speciation and partitioning

Acetic acid is highly soluble in water (LMC 2014). If discharged into waters under typical environmental conditions, acetic acid will be present primarily as the acetate conjugate base anion in the water compartment. However, the chemistry of the receiving water compartment, such as its pH and the presence of metal ions, may affect the speciation and partitioning of this chemical.

2.5.2 Persistence

Acetic acid is readily biodegradable, attaining 74% in 14 days in an experiment conducted according to OECD Test Guideline 301C (LMC 2014). The chemical is therefore not considered to be persistent in the environment according to domestic hazard criteria (EPHC 2009).

2.5.3 Bioaccumulation

Acetic acid has a low measured octanol-water partition coefficient, indicating low potential to bioaccumulate. The chemical is a fundamental component of metabolic cycles and typical internal concentrations will be regulated by normal homeostatic controls. The chemical is not considered to be bioaccumulative according to domestic hazard criteria (EPHC 2009).

2.5.4 Transport

Acetic acid is produced and cycled through ecosystems in a variety of natural biogeochemical processes, including fermentation, hydrolysis, and photolysis. It is an important component of the global carbon cycle, and is transported through rainfall and river systems (Keene and Galloway 1988; Wetzel 2001).

2.6 Environmental effects summary

2.6.1 Critical environmental effects

2.6.1.1 Acute toxicity endpoints for aquatic organisms

The following representative measured median effective concentration (EC50) and median lethal concentration (LC50) values for model organisms were identified for acetic acid:

Taxon	Endpoint	Method
Fish	96h LC50 = 79 mg/L	Experimental *Pimephales promelas* (LMC 2014)
Invertebrates	48h EC50 = 32 mg/L	Experimental *Ampelisca abdita* (LMC 2014)
Algae	Not available	

The majority of the large amount of measured ecotoxicological data available for acetic acid indicates that the chemical is not harmful to aquatic organisms at concentrations above 100 mg/L.

2.6.1.2 Chronic toxicity endpoints for aquatic organisms

No relevant chronic toxicity data for acetic acid or sodium acetate were identified. Acetate is ubiquitous in natural water and acts as a key nutrient, and therefore background concentrations of the chemical are not expected to pose a chronic hazard.

2.7 Categorisation and other characteristics of concern

2.7.1 PBT categorisation

Sodium acetate is not a PBT substance according to domestic environmental hazard criteria.

2.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for this chemical.

2.8 Screening assessment

2.8.1 Assessment

At neutral pH, dissolution of sodium acetate will typically result in the release of sodium and acetate ions to the environment. Both of these chemical species are naturally occurring and ubiquitous in the aquatic environment, and they have low toxicity under typical environmental conditions. In addition, acetate is readily biodegraded and not bioaccumulative, and functions as a key nutrient for many algae and bacteria species.

Release of significant volumes of sodium acetate to aquatic ecosystems may cause temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations or pH changes. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate fluctuations in the concentrations of this key nutrient in aquatic ecosystems. Spills of larger volumes of sodium acetate are expected to be cleaned up before this chemical can be released to surface waters.

2.9 Outcome

A Tier 1 assessment of the environmental risks from the use of sodium acetate is not required.

2.10 References

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3 Choline chloride

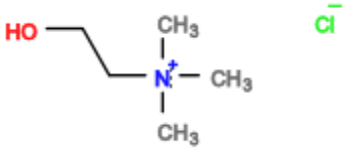
3.1 Background

Ethanaminium, 2-hydroxy-*N*,*N*,*N*-trimethyl-, chloride (or choline chloride) is a 1:1 salt of choline (the 2-hydroxyethyl trimethylammonium cation) and the chloride anion (OECD 2004). Choline occurs naturally in fungi, hops and kingcups (Zeisel et al. 1983). The most abundant source of choline is the head group of lipids in eukaryotic cells (Wargo 2013). It is considered to be an essential nutrient in bacteria, humans and other animals (National Research Council 1998; OECD 2004; Wargo 2013).

Choline chloride is widely used as a food flavouring and nutrient, mostly in animal husbandry (Nordic Council of Ministers 2014; OECD 2004). In the coal seam gas industry, the chemical is used as a clay stabiliser to prevent clays from swelling or shifting (FracFocus 2015). Clay swelling can result in instability of boreholes and a reduction in the permeability of rock formations which contain high proportions of swellable clays (Stringfellow et al. 2014). There is increasing use of choline chloride in hydraulic fracturing as an alternative to the historically used sodium chloride and potassium chloride salts as it is more effective at reducing clay swelling at lower concentrations, and because it is biodegradable (McCurdy 2011; Balchem Corporation 2010; Stringfellow et al. 2014).

Large volumes of choline chloride released to aquatic ecosystems may be a source of physico-chemical stress for local organisms as a result of the increased load of dissolved organic carbon. For example, rapid biodegradation of the chemical may decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life (Stringfellow et al. 2014). However, numerous natural biogeochemical mechanisms exist which tend to limit moderate fluctuations in nutrient levels, which occur frequently in healthy aquatic ecosystems.

3.2 Chemical name and identification

CAS Name	**Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl-, chloride (1:1)**
CAS RN	67-48-1
AICS name	Ethanaminium, 2-hydroxy-*N,N,N*-trimethyl-, chloride
Synonyms	Choline chloride
Structural formula	
Molecular formula	$C_5H_{14}ClNO$
Molecular weight	139.63 g/mol
SMILES	C[N+](C)(C)CCO.[Cl-]

3.3 Physico-chemical properties

Properties	
Physical form	White crystalline solid
Melting point	305°C (dec.) (LMC 2014)
Boiling point	Not applicable due to decomposition on heating (OECD 2004)
Water solubility	650 g/L (OECD 2004)
pK_a	Not available
Log K_{ow}	-3.77 (OECD 2004)
Vapour pressure	6.57×10^{-8} Pa (estimated) (US EPA 2008)

3.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for choline chloride:

Pre-assessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC	No
EDC (Europe)	No

3.5 Environmental fate summary

3.5.1 Dissolution, speciation and partitioning

Choline chloride is highly water soluble and non-volatile. When released to water under typical environmental conditions, the quaternary ammonium salt dissociates to release a positively charged choline ion and a negatively charged chloride ion (OECD 2004). While the choline cation can adsorb to clays and natural organic materials, such as humic substances (Games et al. 1982), it is unlikely to partition to the atmosphere based on its low volatility (OECD 2004). Consequently, choline is expected to exist mainly in the soil, sediment and water compartments. The environmental fate of the naturally ubiquitous chloride ion is not considered in this report.

3.5.2 Persistence

Choline chloride is Not Persistent (Not P). Based on a ready biodegradability test, 93% biodegradation was attained in 14 days in a MITI-I test conducted according to OECD-criteria (MITI 1992). Hence, the chemical is determined to be readily biodegradable.

3.5.3 Bioaccumulation

Choline chloride is Not Bioaccumulative (Not B). Choline chloride has a low measured octanol-water partition coefficient (OECD 2004), which typically indicates a low potential to accumulate in organisms. Furthermore, choline is an essential nutrient in bacteria, humans and other animals (National Research Council 1998; OECD 2004; Wargo 2013). Dietary choline is absorbed by the gut or metabolised by bacteria to form betaine and methylamines (Zeisel et al. 1983). It functions as a precursor for acetylcholine, phospholipids, and the methyl donor betaine and is important for the structural integrity of cell membranes, methyl metabolism, cholinergic neurotransmission, transmembrane signaling, and lipid and cholesterol transport and metabolism (Zeisel 2000).

3.5.4 Transport

Choline chloride is a salt which dissociates in water to release the naturally occurring and globally distributed ions, choline and chloride. Based on its low potential to partition to the atmosphere and observed ready biodegradation, the chemical is not expected to undergo long-range transport.

3.6 Environmental effects summary

3.6.1 Critical environmental effects

3.6.1.1 Acute toxicity endpoints for aquatic organisms

The median lethal concentration (LC50) and median effective concentration (EC50) values for model organisms across three trophic levels were obtained from databases in the OECD QSAR Toolbox (LMC 2014) and are used to characterise the acute effects of this chemical:

Taxon	Endpoint	Method
Fish	96 h LC50 > 10 000 mg/L	Experimental *Leuciscus idus* (LMC 2014)
Invertebrates	48 h EC50 = 350 mg/L	Experimental *Daphnia magna* (LMC 2014)
Algae	96 h EC50 > 500 mg/L	Experimental *Scenedesmus subspicatus* (LMC 2014)

The large amount of measured aquatic ecotoxicological data available for this chemical indicates that choline chloride is unlikely to be harmful to aquatic organisms.

3.6.1.2 Chronic toxicity endpoints for aquatic organisms

The following No-Observed-Effect-Concentration (NOEC) values for model organisms from two major trophic levels were obtained from databases in the OECD QSAR Toolbox (LMC 2014) and used to characterise the chronic effects of this chemical:

Taxon	Endpoint	Method
Fish	Not available	-
Invertebrates	21 d NOEC = 30 mg/L	Experimental *Daphnia magna* (LMC 2014)
Algae	72 h NOEC = 32 mg/L	Experimental *Pseudokirchneriella subcapitata* (LMC 2014)

Available chronic toxicity data indicate that choline chloride is unlikely to have long-term harmful effects on aquatic organisms.

3.7 Categorisation and other characteristics of concern

3.7.1 PBT categorisation

The chemical is not a PBT substance according to domestic environmental hazard criteria.

3.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for this chemical.

3.8 Screening assessment

3.8.1 Assessment

Choline is an essential nutrient in bacteria, humans and other animals. Under environmental conditions, choline chloride dissociates to release choline and chloride ions, which are ubiquitous in the environment. Choline chloride is readily biodegradable and not bioaccumulative, and it has low toxicity to aquatic organisms in both short-term and long-term exposures.

Large volumes of choline chloride abruptly released to aquatic ecosystems may cause temporary physico-chemical stress for local organisms, such as decreased dissolved oxygen concentrations. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate fluctuations in the concentrations of choline in aquatic ecosystems. Spills of larger volumes of choline chloride are expected to be cleaned up before this chemical can be released to surface waters.

3.9 Outcome

A Tier 1 assessment of the environmental risks from the use of choline chloride is not required.

3.10 References

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Zeisel, SH, Wishnok, JS and Blusztajn, JK 1983, 'Formation of methylamines from ingested choline and lecithin', *Journal of Pharmacology and Experimental Therapeutics*, vol. 225, pp. 320-324.

Zeisel, SH 2000, 'Choline: an essential nutrient for humans', *Nutrition*, vol. 16, pp. 669-671.

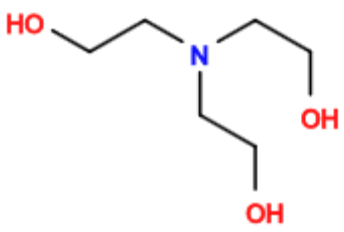
4 Triethanolamine

4.1 Background

Ethanol, 2,2',2''-nitrilotris (or triethanolamine) is a high volume industrial chemical that has a wide range of industrial and domestic uses including in the manufacture of surfactants, emulsifiers and dispersing agents, in lubricating/metal work applications, and in cosmetics (OECD 1995; Nordic Council of Ministers 2014). In the coal seam gas industry, the chemical is a component of gelling agents used in hydraulic fracturing fluids. The specific function identified for triethanolamine is gel management (EHP QLD 2013). Gelling agents increase the viscosity of fracturing fluids, allowing for better proppant suspension and transport into developed fractures (Stringfellow et al. 2014).

Triethanolamine is an organic base that is moderately basic in aqueous solution. Direct release of large volumes of triethanolamine to a natural water body has some potential to cause physico-chemical stress to aquatic organisms by temporarily increasing the pH above the normal range. However, triethanolamine is inherently biodegradable, has low toxicity to aquatic organisms and does not bioaccumulate. Hence, no long-term adverse effects would be expected from uncontained direct releases to water or soil. Diffuse low-level emissions of triethanolamine to soil or water are not expected to pose a concern to the environment.

4.2 Chemical name and identification

CAS Name	**Ethanol, 2,2',2''-nitrilotris-**
CAS RN	102-71-6
AICS name	Ethanol, 2,2',2''-nitrilotris-
Synonyms	Triethanolamine TEA
Structural formula	
Molecular formula	$C_6H_{15}NO_3$
Molecular weight	149.19 g/mol
SMILES	C(O)CN(CCO)CCO

4.3 Physico-chemical properties

Properties	
Physical form	Liquid (at 25°C)
Melting point	20.5°C (LMC 2014)
Boiling point	335°C (LMC 2014)
Density (relative to water)	1.12 (OECD 1995)
Water solubility	1000 g/L (LMC 2014)
pK_a	7.76 (Dissociation of the triethanolammonium species in water; LMC 2014)
Log K_{ow}	-1.0 (LMC 2014)
Vapour pressure	0.000479 Pa (LMC 2014)

4.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for triethanolamine:

Pre-assessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

4.5 Environmental fate summary

4.5.1 Dissolution, speciation and partitioning

Triethanolamine is a highly water soluble organic base that is moderately basic based on the measured acid dissociation constant for the triethanolammonium ion in water (pK_a = 7.76). Hence, if released directly into natural water bodies, triethanolamine will exist in both protonated and neutral forms, the relative proportions of which will depend on the pH of the water body (OECD 1995).

If released to soil, volatilisation is not considered to be an important fate process based on the low volatility of triethanolamine (OECD 1995). The neutral form of the chemical may be mobile in soil based on the estimated soil adsorption coefficient (K_{oc} = 3 L/kg). The soil mobility of the triethanolammonium cation may be lower than for the free base due to specific interactions with minerals and organic matter in soil (OECD 1995).

4.5.2 Persistence

Triethanolamine is categorised as Persistent (P) according to domestic hazard criteria. This conservative categorisation was adopted because there are conflicting findings from standard ready biodegradability tests regarding the rate of biodegradation of triethanolamine. Some studies indicate relative rapid biodegradation, whereas some closed bottle studies indicate slow biodegradation under the test conditions (OECD 1995). However, the chemical is inherently biodegradable. The results of a test using OECD test guideline 302B showed that 89% of the chemical is degraded after 14 days (OECD 1995).

4.5.3 Bioaccumulation

Triethanolamine is Not Bioaccumulative (Not B) according to domestic hazard criteria. Based on a measured bioconcentration factor of less than 3.9 L/kg in fish, triethanolamine has a low bioaccumulation potential in aquatic organisms (LMC 2014). This finding is consistent with the high water solubility and low measured octanol-water partition coefficient (log K_{ow} = -1.0) for triethanolamine.

4.5.4 Transport

Based on its low potential to partition to the atmosphere and its ultimate biodegradability, triethanolamine is not expected to undergo long-range transport.

4.6 Environmental effects summary

4.6.1 Critical environmental effects

Only studies where test media were neutralised were considered for this assessment, to most closely represent potential for toxicity under typical environmental conditions.

At neutral pH, triethanolamine will exist in both protonated and neutral forms. The protonated and neutral forms of the chemical may have different toxicity properties in aquatic organisms. However, when pH moves beyond the normal range for environmental water, toxic effects may occur as a result of this physico-chemical stress rather than an ecotoxic effect of the chemical. Therefore, it is not possible to determine if toxic effects observed significantly beyond neutral pH are as a result of physico-chemical stress or differing toxicity characteristics between protonated and neutral forms of the chemical.

4.6.1.1 Acute toxicity endpoints for aquatic organisms

The median lethal concentration (LC50) and median effective concentration (EC50) values for model organisms across three trophic levels were used to characterise the acute effects of this chemical:

Taxon	Endpoint	Method
Fish	96 h LC50 = 11 800 mg/L	Experimental Pimephales promelas (OECD 1995) pH = 7.8
Invertebrates	24 h EC50 = 1390 mg/L	Experimental *Daphnia magna* (OECD 1995) pH = 7.6-7.7

Taxon	Endpoint	Method
Algae	96 h EC50 = 910 mg/L	Experimental *Scenedesmus subspicatus* (OECD 1995) Test media neutralised

The large amount of measured aquatic ecotoxicological data available for this chemical indicates that triethanolamine is unlikely to be harmful to aquatic organisms.

4.6.1.2 Chronic toxicity endpoints for aquatic organisms

The following No-Observed-Effect-Concentration (NOEC) values for model organisms from two major trophic levels were obtained from databases in the OECD QSAR Toolbox (LMC 2014) and used to characterise the chronic effects of this chemical:

Taxon	Endpoint	Method
Fish	Not available	-
Invertebrates	21 d NOEC = 16 mg/L	Experimental *Daphnia magna* (ECHA 2015) pH = 7.6-7.7
Algae	7-8 d NOEC = 1.8 mg/L	Experimental *Scenedesmus quadricauda* (OECD 1995) Test media neutralised

Available chronic toxicity data indicates that triethanolamine is unlikely to be harmful to aquatic organisms through long-term exposure.

4.7 Categorisation and other characteristics of concern

4.7.1 PBT categorisation

Triethanolamine is not a PBT substance according to domestic environmental hazard criteria.

4.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for this chemical.

4.8 Screening assessment

4.8.1 Assessment

Triethanolamine is an organic base that exists as a mixture of neutral and protonated forms in surface waters. The protonation of triethanolamine is an acid-base reaction that has the potential to change the pH of the receiving water body depending on the volume of triethanolamine introduced and the natural buffering capacity of the water body. Direct release of large volumes of triethanolamine to a natural water body therefore has some potential to cause physico-chemical stress to aquatic organisms by temporarily increasing the pH above the normal range. However, triethanolamine is inherently biodegradable, has low toxicity to aquatic organisms and does not bioaccumulate. Hence, no long-term adverse

effects would be expected from uncontained direct releases to water or soil. Furthermore, spills of large volumes of triethanolamine are expected to be cleaned up before this chemical can be released to surface waters.

Diffuse low-level emissions of triethanolamine to soil or water are not expected to pose a concern to the environment based on the low toxicity and biodegradability of triethanolamine in surface waters.

4.9 Outcome

A Tier 1 assessment of the environmental risks from the use of triethanolamine is not required.

4.10 References

ECHA 2015, *Registered substances database,* available at <http://echa.europa.eu/information-on-chemicals/registered-substances>.

EHP QLD 2013, *Chemicals used in fraccing,* Department of Environment and Heritage protection Queensland Government, available at <https://www.ehp.qld.gov.au/management/non-mining/fraccing-chemicals.html>.

LMC 2014, The OECD QSAR Toolbox for grouping chemicals into categories, v 3.2 Bourgas, Bulgaria.

Nordic Council of Ministers 2014, *Substances in preparations in nordic countries SPIN, Copenhagen, Denmark*, available at <http://fmp.spin2000.net/fmi/xsl/spin/SPIN/maininfo.xsl?-db=SPINstof&casnr.op=eq&casnr=102-71-6&-max=1&-lay=SPINnavn&-find>.

OECD 1995, OECD existing chemicals database. Organisation for Economic Cooperation and Development, Williamsburg, Virginia, available at <http://webnet.oecd.org/Hpv/UI/SIDS_Details.aspx?id=CEF02D50-2294-462B-8027-FB4EC67D5D81>.

Stringfellow, WT, Domen, JK, Camarillo, MK, Sandelin, WL, and Borglin, S 2014, 'Physical, chemical, and biological characteristics of compounds used in hydraulic fracturing', *Journal of Hazardous Materials*, vol. 275, pp. 37-54.

5 Tetrasodium EDTA

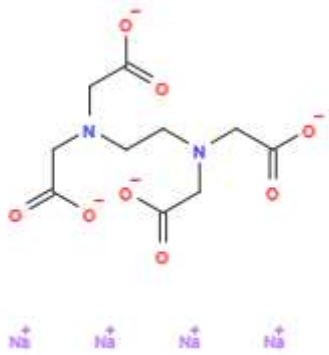
5.1 Background

Glycine, *N*, *N′*-1,2-ethanediylbis [*N*-(carboxymethyl)-, tetrasodium salt (tetrasodium ethylenediaminetetraacetic acid; tetrasodium EDTA) is a strong chelating agent, and can form complexes with many metal ions (Nowack et al. 2001). It has uses in a wide range of industrial and domestic applications, including household and commercial detergents, textile finishing and paper processing. In the coal seam gas industry, tetrasodium EDTA is used for iron control. Iron is naturally abundant in the environment and is a key nutrient for plants and animals, but can form problematic precipitates in coal seam gas operations (ANZECC and ARMCANZ 2000; Frenier et al 2003).

Ethylenediaminetetraacetic acid (EDTA) is a synthetic aminocarboxylic acid polydentate ligand with a strong affinity for a range of metal ions. Release of uncomplexed EDTA to aquatic ecosystems can cause moderate indirect ecotoxicity effects due to its ability to sequester essential trace metals (e.g., zinc(II) and copper(II)). However, EDTA is typically released to the environment in the form of metal complexes, as its chelating action is the functionally relevant characteristic. When complexed to nutrient metals, the toxicity of EDTA is low (Nowack et al. 2001; ECB 2004).

As a result of its extensive industrial use, EDTA is routinely detected in environmental waters at concentrations between 0.1 and 1 mg/L (ECB 2004). These background concentrations have previously been identified as of concern, as this may allow mobilisation of toxic heavy metals in contaminated aquatic ecosystems (Nowack 2002; ECB 2004). However, further studies have concluded that significant remobilisation of existing contaminants is only expected to occur in extreme cases when high volumes of EDTA are released (Nowack et al 2001; ECB 2004).

5.2 Chemical name and identification

CAS Name	**Glycine, *N*, *N′*-1,2-ethanediylbis [*N*-(carboxymethyl)-, sodium salt (1:4)**
CAS RN	64-02-8
AICS name	Glycine, *N*, *N′*-1,2-ethanediylbis [*N*-(carboxymethyl)-, tetrasodium salt
Synonyms	Tetrasodium EDTA Tetrasodium ethylenediaminetetraacetic acid
Structural formula	
Molecular formula	$C_{10}H_{12}N_2Na_4O_8$

CAS Name	**Glycine, *N*, *N'*-1,2-ethanediylbis [*N*-(carboxymethyl)-, sodium salt (1:4)**
Molecular weight	380.17 g/mol
SMILES	C(=O)([O-])CN(CC(=O)[O-])CCN(CC(=O)[O-])CC(=O)[O-].[Na+].[Na+].[Na+].[Na+]

5.3 Physico-chemical properties

Properties	
Melting point	>300.0 °C (LMC 2014)
Boiling point	Not available
Water solubility	500 g/L (LMC 2014)
pK_a	pK_{a1} = 1.95 pK_{a2} = 2.68 pK_{a3} = 6.11 pK_{a4} = 10.17 (Butler 1998)
Log K_{ow}	Not available
Vapour pressure	Not available

5.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for tetrasodium EDTA.

5.5 Environmental fate summary

5.5.1 Dissolution, speciation and partitioning

EDTA is typically released to the environment in its complexed form (Nowack et al. 2001). The speciation of metal complexes is determined by the complex released, and metal exchange reactions mediated by its interactions with the chemistry of the receiving water compartment (Nowack 2002; ECB 2004). However, complexes of EDTA with iron(III) are often detected in river water due to the ubiquity of iron(III) and the slow kinetics of relevant metal exchange reactions (half life approximately 20 days) (Nowack 2002).

Partitioning of complexed EDTA between water and sediment compartments is dependent on the metal ion complexed. For example, EDTA complexed with cobalt(III) and iron(III) partitions predominately to the water compartment, while lead(II) EDTA complexes adsorb strongly to sediment (Nowack 2002).

5.5.2 Persistence

EDTA is not readily biodegradable. Various studies conducted to standardised ready biodegradation test guidelines have found biodegradation to range between 0% and 10% in 28 days. The chemical is also resistant to hydrolysis (ECB 2004; NITE 2015). The chemical is considered to be persistent in the environment according to domestic hazard criteria (EPHC 2009).

However, EDTA is photolytically unstable when complexed with iron(III) ions. The complex is reported to have a half life of 5 hours in central Europe in summer, with a worst-case half life of 20 days. A number of degradation products are expected, which are expected to be inherently biodegradable (ECB 2004).

5.5.3 Bioaccumulation

Measured bioconcentration factors available for EDTA in fish are less than 15 L/kg (ECB 2004; NITE 2015), indicating low potential to bioaccumulate. The chemical is not considered to be bioaccumulative according to domestic hazard criteria (EPHC 2009).

5.5.4 Transport

Environmental transport of EDTA will be determined by the metal ions it is complexed with. Most studies investigating the transport of EDTA complexes compare this to transport of the uncomplexed metal. Generally, EDTA is found to decrease adsorption of metals and therefore increase its potential for transport in the environment (ECB 2004).

5.6 Environmental effects summary

5.6.1 Critical environmental effects

The toxicity of complexing agents is determined by the presence of metal ions and other factors affecting speciation, such as pH. The chemical is most toxic to aquatic organisms when released to the environment uncomplexed. When uncomplexed, EDTA chelates key nutrients from ecosystems and causes nutrient deficiency (ECB 2004). Available ecotoxicity data indicate that uncomplexed EDTA is not toxic according to domestic hazard criteria (EPHC 2009). However, assuming at least stoichiometric amounts of nutrients are present, actual toxicity in the environment is expected to be lower (ECB 2004).

5.6.1.1 Acute toxicity endpoints for aquatic organisms

The following measured median effective concentration (EC50) and median lethal concentration (LC50) values for model organisms were identified for EDTA. Studies were conducted in accordance with OECD test guidelines. No modification of test media to increase nutrient concentrations was reported:

Taxon	Endpoint	Method
Fish	96 h LC50 = 74 mg/L	Experimental *Oryzias latipes* (NITE 2015)
Invertebrates	48 h EC50 = 57 mg/L	Experimental *Daphnia magna* (NITE 2015)
Algae	72 h EC50 = 6 mg/L	Experimental *Pseudokirchneriella subcapitata* (NITE 2015)

5.6.1.2 Chronic toxicity endpoints for aquatic organisms

The following no-observed-effect concentration (NOEC) values for model organisms were identified for EDTA. Studies were conducted in accordance with OECD test guidelines. No modification of test media to increase nutrient concentrations was reported:

Taxon	Endpoint	Method
Fish	35 d NOEC > 26 mg/L	Experimental *Danio rerio* (ECB 2004)
Invertebrates	21 d NOEC = 5.5 mg/L	Experimental *Daphnia magna* (NITE 2015)
Algae	72 h NOEC = 0.32 mg/L	Experimental *Pseudokirchneriella subcapitata* (NITE 2015)

5.7 Categorisation and other characteristics of concern

5.7.1 PBT categorisation

The chemical is not a PBT substance according to domestic environmental hazard criteria.

5.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for this chemical.

5.8 Screening assessment

5.8.1 Assessment

Tetrasodium EDTA is a common chelating agent, and is released to the environment as a result of a wide number of domestic and industrial uses. Metal complexes of EDTA are consequently routinely detected in the environment. Due to its potential to modify the behaviour of metals in the environment, EDTA has previously been identified as of potential concern internationally.

Use of tetrasodium EDTA in coal seam gas is expected to result in the formation of EDTA metal complexes, most likely with iron(III). Some EDTA complexes with heavy metals and radionuclides could also be formed, resulting in the mobilisation of these species. However, these potential indirect effects are beyond the scope of this assessment.

Release of EDTA complexed with metals such as iron(III) to the environment will have limited direct ecotoxic effects. Metal exchange reactions may result in the mobilisation of heavy metal contaminants, if present in the receiving compartment. However, the potential for this to occur is expected to be limited, given the slow kinetics of metal exchange reactions for the iron(III) EDTA complex and the photolytic half life of this compound.

Accidental spills of tetrasodium EDTA during transport to coal seam gas operations could result in release of significant quantities of uncomplexed EDTA to the environment. Although large quantities of uncomplexed EDTA could mobilise heavy metal contaminants and/or sequester key nutrients in aquatic ecosystems, such impacts are not expected to occur before clean-up of accidental spills can occur.

5.9 Outcome

A Tier 1 assessment of the environmental risks from the use of tetrasodium EDTA is not required.

5.10 References

ANZECC and ARMCANZ 2000, Australia and New Zealand Environment and Conservation Council and Agriculture and Resource Management Council of Australia and New Zealand 2000, Australian and New Zealand Guidelines for Fresh and Marine Water Quality (Vol. 1), Australian Water Association, Artarmon, NSW.

Butler, JN 1998, *Ionic equilibrium: solubility and pH calculations*, John Wiley and Sons, New York, USA.

ECB 2004, *European Union risk assessment report for tetrasodium ethylenediaminetetraacetate,* available at <http://echa.europa.eu/documents/10162/415c121b-12cd-40a2-bd56-812c57c303ce>.

EPHC 2009, *Environmental risk assessment guidance manual for industrial chemicals*, Environment Protection and Heritage Council, Canberra, retrieved from <http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals>.

Frenier, WW, Rainey, M, Wilson, D, Crump, D and Jones, L 2003, A biodegradable chelating agent is developed for stimulation of oil and gas formations', presented at *Exploration and production environmental conference*, 10-12 March, San Antonio, Texas.

LMC 2014, *The OECD QSAR toolbox for grouping chemicals into categories, v 3.1.,* Laboratory of Mathematical Chemistry, University "Prof. Dr. Assen Zlatarov", Burgas, Bulgaria, retrieved from <http://oasis-lmc.org/>.

NITE 2015, *Japan chemicals collaborative knowledge database*, National Institute of Technology and Evaluation, Tokyo, available at <http://www.safe.nite.go.jp/jcheck/top.action;jsessionid=2EAC29067591B266CC34B9196E5BEC46?request_locale=en>.

Nowack, B 2002, 'Environmental chemistry of aminopolycarboxylate chelating agents', *Environmental Science and Technology*, vol. 36(19), pp. 4009-4016.

Nowack, B, Kari, FG, Krüger and HG 2001, 'The remobilization of metals from iron oxides and sediments by metal-EDTA complexes', *Water, Air and Soil Pollution*, vol. 125, pp. 243-257.

6 Water

Water has been assigned registry number 7732-18-5 by the Chemical Abstracts Service. This CAS RN has been taken to indicate the pure chemical substance, water (i.e., H_2O). It has not been taken to include natural or treated surface water which is used in the coal seam gas industry. Water is present as the dominant constituent of aqueous solutions and slurries used in hydraulic fracturing operations.

Water is essential for all life and is not considered to be an ecotoxicological hazard. No further assessment is required.

7 Terpenes

Confidentiality from public disclosure was claimed for the name and Chemical Abstracts Service Registry Number (CAS RN) of this chemical. Information about the chemical subject to commercial-in-confidence claims was provided to the assessment team and a detailed screening assessment of the chemical was conducted. The chemical is referred to as the 'substance' hereafter.

7.1 Background

The substance is reported to be composed of a number of naturally occurring terpenes (US EPAa). Naturally occurring terpenes are found in plants and are often noted for their fragrance and flavouring properties. Well-known terpenes include those found in pine trees, citrus fruits, lavender flowers and rosemary leaves (Breitmier 2006). Industrially, terpenes are used in perfumes, cosmetics, soaps, detergents, and other cleaning products (US EPAa). In the Australian coal seam gas industry, the substance is reported to be used as a surfactant, solvent, and dispersant in hydraulic fracturing or pre-treatment formulations.

Due to their high volatility, terpenes released from plants typically occur naturally in the air compartment (US EPAa). As a component of plants, background concentrations are also expected to occur in water and soil compartments. However, these concentrations will be limited by the low water solubility and high biodegradability of these substances. At higher concentrations, terpenes are known to cause toxic effects in aquatic organisms. For one terpene, acute median lethal effect concentration (LC50) values in fish and aquatic invertebrates are reported to be less than 1 mg/L (NICNAS).

7.2 Chemical name and identification

The substance is an unknown or variable composition, a complex product of a chemical reaction, or a biological material (UVCB) substance (US EPAb).

CAS Name	**CBI**
CAS RN	CBI

7.3 Physico-chemical properties

The below measured data were identified for the UVCB substance, or based on measured data for major components of the substance (ECHA 2015):

Property	
Physical form	Liquid (US EPAb)
Melting point	< -80°C (ECHA 2015)
Boiling point	175.7°C (ECHA 2015)
Water solubility	< 10 mg/L (ECHA 2015)
pKa	Not applicable. The component chemicals do not contain readily ionizable function groups.
Log Kow	3.7-4.5 (ECHA 2015)

Vapour pressure	> 101 Pa (ECHA 2015)

7.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for the substance:

Pre-assessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

7.5 Environmental fate summary

7.5.1 Dissoluion, speciation and partitioning

The substance is slightly soluble and highly volatile. A major constituent of this substance is expected to be highly volatile from water and partition primarily to the atmosphere, based on a Henry's Law constant of 34 800 Pa m^3/mol (NICNAS). Based on its high octanol-water partition coefficient, this component may also experience moderate adsorption to sediment if released to the aquatic environment. If released to the terrestrial environment, the component is expected to have low to very low mobility, with volatilisation potentially inhibited by strong adsorption (NICNAS).

Based on this information, the component chemicals of this substance are expected to partition predominantly to the atmosphere, soil and sediment.

7.5.2 Persistence

The substance is readily biodegradable, attaining 81% biodegradation in 28 days in an OECD Test Guideline 301D study (ECHA 2015). The substance is not considered to be persistent according to domestic hazard criteria (EPHC 2009).

In the atmosphere, the component chemicals of this substance are expected to be rapidly degraded through reactions with hydroxyl radicals (US EPAb). A daytime atmospheric half-life of 12 to 48 minutes has previously been estimated for a major component of the chemical based on indirect photo-oxidation reactions (NICNAS).

7.5.3 Bioaccumulation

No measured bioaccumulation data are available for the substance or any of its major component chemicals. A previous assessment of a major component concluded that this chemical may have some potential to bioaccumulate (NICNAS). This is consistent with the high octanol-water partition coefficient for the component. However, terpenes occur naturally

in the foods of many animals, and are metabolised to polar metabolites via the cytochrome P450 pathway (US EPAa). This is expected to limit the bioaccumulation potential. A more recent assessment has concluded that the substance has only low to moderate bioaccumulation potential (US EPAb).

Based on the available information, the bioaccumulation potential of the substance is assessed as Uncertain (i.e., Uncertain B) according to domestic hazard criteria (EPHC 2009).

7.5.4 Transport

Long-range transport of the substance (or its component chemicals) in the environment is expected to be limited based on its low water solubility, and the rapid degradation of the component chemicals in the atmosphere.

7.6 Environmental effects summary

7.6.1 Critical environmental effects

7.6.1.1 Acute toxicity endpoints for aquatic organisms

The following representative measured LC50, median effective concentration (EC50) and median effective loading concentration (EL50) values for model organisms were identified for the substance. Based on these findings, the substance is not considered to be toxic according to domestic hazard criteria (EPHC 2009):

Taxon	Endpoint	Method
Fish	96 h LC50 = 5.07 mg/L	Experimental *Danio rerio* (ECHA 2015)
Invertebrates	48 h EL50 = 2.1 mg/L	Experimental *Daphnia magna* (ECHA 2015)
Algae	72 h EC50 = 4.8 mg/L	Experimental *Pseudokirchneriella subcapitata* (ECHA 2015)

The substance has a variable composition. Therefore, it should be noted that the above reported toxicity values may underestimate toxicity if more toxic components are present in higher proportions (NICNAS).

7.6.1.2 Chronic toxicity endpoints for aquatic organisms

No relevant chronic toxicity data were identified for the substance.

7.6.1.3 Acute toxicity endpoints for terrestrial organisms

Toxicity data available for a major component of the substance indicate potential for some acute toxic effects in soil fauna (NICNAS).

7.7 Categorisation and other characteristics of concern

7.7.1 PBT categorisation

The substance is not a PBT substance according to domestic environmental hazard criteria.

7.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for this substance.

7.8 Screening assessment

7.8.1 Assessment

The substance is composed primarily of simple terpenes. Terpenes occur naturally in plants and are widely distributed in the environment, particularly in the air compartment. If released to the terrestrial environment, the component chemicals of the substance are expected to undergo volatilisation or rapid biodegradation. Strong sorption of the component chemicals to soil may limit these processes. However, if these processes are inhibited by strong sorption, the bioavailability of the component chemicals to cause toxic effects is expected to be similarly restricted. Any toxic effects that do occur will be localised due to the immobility of the component chemicals. Runoff to surface waters is not expected. If released directly to surface waters, the component chemicals of this substance are expected to predominately volatilise to the atmosphere, or partition to sediment. Therefore, the potential for significant exposure to aquatic organisms is low.

The bioaccumulation potential of the substance has been conservatively categorised as Uncertain based on the lipophilicity of major component chemicals. However, bioaccumulation of the component chemicals of this substance is not currently considered to pose a concern based on the ubiquity of these chemicals in the environment, and their known susceptibility to bio-elimination processes in animals.

7.9 Outcome

A Tier 1 assessment of the environmental risks from the use of the substance is not required.

7.10 References

ECHA 2015, *Registered substances database*. Helsinki, Finland, available at <http://echa.europa.eu/information-on-chemicals/registered-substances>.

EPHC 2009, *Environmental risk assessment guidance manual for industrial chemicals*, Environment Protection and Heritage Council, Canberra, retrieved from <http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals>.

NICNAS *Chemical assessment report*. Sydney, Australia.

US EPAa *Revised test plan*. Washington DC, USA.

US EPAb Screening-level hazard categorisation. Washington DC, USA.

8 Alkanes, C_{12-26} – branched and linear

8.1 Background

Alkanes, C_{12-26}-branched and linear, hereafter referred to as 'the substance', is an unknown or variable composition, complex reaction products or biological materials (UVCB) substance. It consists of a mixture of linear and branched alkanes. Alkanes with between 12 and 26 carbon atoms have many uses including as fuel for domestic heating (EC and HC 2015a). They are also used as solvents, chemical intermediates, in gasoline, as fuels in furnaces, burners and engines (US NLM 2013), and in non-aqueous drilling muds.

In the coal seam gas industry, petroleum distillates are sometimes pumped into wells under high-pressure instead of aqueous based fluids. This may be done so that higher concentrations of polymers can be injected. Petroleum distillates may also be used as carrier fluids for dissolving additives before mixing, in what are otherwise aqueous hydraulic fracturing treatments (Strongfellow et al. 2014). It has been reported the substance is used as a gelling agent during fracturing or fracturing pretreatment.

Release of large volumes of the substance to natural waterways may disturb the health of aquatic ecosystems through direct and indirect physical and chemical effects. For example, petroleum products are known to affect aquatic birds through eliminating insulation and water repellency of their feathers, water logging, hypothermia and ingestion of the chemicals while preening (EC and HC 2015a). Further, rapid biodegradation of large quantities of the substance in natural water bodies may decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate concentrations of the substance in aquatic ecosystems.

8.2 Chemical name and identification

CAS Name	**Alkanes, C_{12-26} -branched and linear**
CAS RN	90622-53-0
AICS name	Not on AICS

8.3 Physico-chemical properties

There was little relevant physico-chemical data available for the substance. Since the substance is a UVCB with variable proportions of linear and branched hydrocarbons, data for the linear components of the substance (C_{12}-C_{26} *n*-alkanes) have been used to give an indication of the expected properties of the substance:

Property	
Physical form	Liquid at standard temperature and pressure (ECHA 2015)
Melting point	-40 to 6°C (ECHA 2015)
Boiling point	172 to 344°C (ECHA 2015)

Property	
Water solubility	0.0037 mg/L (Measured, $C_{12}H_{26}$) (US EPA 2008) 0.000076 mg/L (Measured, $C_{15}H_{32}$) (US EPA 2008) 0.006 mg/L (Measured, $C_{18}H_{38}$) (US EPA 2008) 0.0017 mg/L (Measured, $C_{26}H_{54}$) (US EPA 2008)
pK_a	No dissociable functions
Log K_{ow}	6.10 (Measured, $C_{12}H_{26}$) (US EPA 2008) 13.11 (Calculated, $C_{26}H_{54}$) (US EPA 2008)
Vapour pressure	400 Pa at 40°C (ECHA 2015) 18 Pa (Measured, $C_{12}H_{26}$) (US EPA 2008) 6.25×10^{-5} Pa (Measured, $C_{26}H_{54}$) (US EPA 2008)

8.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for the substance:

Pre-assessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

8.5 Environmental fate summary

8.5.1 Partitioning

The substance is expected to have very low solubility in water based on data available for the representative *n*-alkanes, with measured water solubilities ranging from 0.076 µg/L (C_{15}) to 6 µg/L (C_{18}). The linear components of the substance have measured vapour pressures ranging from 6.25×10^{-5} Pa (C_{26}) to 18.0 Pa (C_{12}). If released to the environment the high vapour pressure components of the substance are expected to partition to air, while the low vapour pressure components are expected to partition to soil or sediment.

The available measured Henry's Law constants for representative *n*-alkanes are high [4.79×10^{4} Pa m^3/ mol (C_{16}) to 1.28×10^{6} Pa m^3/mol (C_{15})] [SRC database, (LMC 2014)] indicating that components of the substance are expected to rapidly partition to air if it is released to water. Components of the substance that do not volatilise from water can form fine dispersions and discrete particles in the water column (EC and HC 2015a).

8.5.2 Persistence

It has been widely demonstrated that nearly all soils and sediments have populations of bacteria and other organisms that are capable of degrading petroleum hydrocarbons. The *n*-alkanes, especially in the C_{10}-C_{25} range, are rapidly degraded. Fuel oils, which are analogues of the substance, are considered to be inherently biodegradable based on their hydrocarbon components (EC and HC 2015a). The proportion of branched alkanes in the substance may reduce its biodegradability since tertiary carbons in an alkyl chain generally reduce the ease of biodegradability (van Leeuwen and Hermens 1995). If the substance is released to the environment it is expected to eventually degrade into water and oxides of carbon.

The substance is a UVCB which contains components with a range of vapour pressures. Dodecane, a linear C_{12} hydrocarbon which is representative of the highest vapour pressure components of the substance, has a calculated half-life in air of 9.2 h due to reaction with hydroxyl radicals according to the AOPWIN Program v1.92 (US EPA 2008). Therefore, the substance is not expected to be persistent in air.

8.5.3 Bioaccumulation

No bioaccumulation data were available for the substance. Most components of the substances are not expected to have high bioaccumulation potential, with data from previous studies indicating that the component of the substance with the highest bioaccumulation potential are the C_{13}-C_{15} branched alkanes (EC and HC 2015a; 2015b). No further data were identified to further evaluate this potential. However, it has previously been hypothesised that these chemicals will not experience significant biomagnification in aquatic or terrestrial food webs largely because a combination of metabolism, low dietary assimilation efficiency and growth dilution allows the elimination rate to exceed the uptake rate from the diet (EC and HC 2015a; 2015b).

8.5.4 Transport

The substance is a UVCB which contains components with a wide range of vapour pressures. The linear C_{12} hydrocarbon, which is representative of the highest vapour pressure components of the substance, has a calculated half-life in air of 9.2 h due to reaction with hydroxyl radicals according to the AOPWIN Program v1.92 (US EPA 2008). Therefore, based on its expected short lifetime in air, the substance is not expected to undergo long-range transport.

8.6 Environmental effects summary

8.6.1 Critical environmental effects

All the components of the substance are profiled as ‘Neutral Organics’ by ECOSAR (US EPA 2012) and ‘Base surface narcotics’ by OECD QSAR Toolbox (LMC 2014).

8.6.1.1 Acute toxicity endpoints for aquatic organisms

No acute ecotoxicity data were available for the substance.

The following measured median lethal loading level (LL50) and median effective loading level (EL50) values for model organisms were identified for representative components of the substance. The endpoints were obtained from databases in the OECD QSAR Toolbox (LMC 2013):

Taxon	Endpoint	Method
Fish	96 h LL50 > 1 000 mg/L	Experimental *Oncorhynchus mykiss* (C11-C14 linear and branched alkanes and cyclics with <2% aromatics)
Invertebrates	48 h EL50 > 1 000 mg/L	Experimental *Daphnia magna* (4 studies on C_{12}, C_{13}, C_{14} and C_{15} linear alkanes)
Algae	72 h EL50 > 1 000 mg/L	Experimental *Skeletonema costatum* (C_{11}-C_{14} linear and branched alkanes and cyclics with <2% aromatics)

The substance is a mixture of linear and branched alkanes with carbon numbers in the range C_{12}-C_{26}. These chemicals are non-ionisable and non-reactive organic compounds which manifest toxicity through simple non-polar narcosis (Mayo-Bean et al 2012). Therefore, the ecotoxicity of the components can be evaluated using standard structure-activity relationships based on log K_{ow} and water solubility (US EPA 2012).

The lowest molecular weight linear component of the substance, dodecane (C_{12}), is predicted to have no ecotoxic effects at saturation to fish, invertebrates and algae based on its high log K_{ow} and low water solubility. The alkanes with carbon numbers C_{13}-C_{26} have increasing log K_{ow} values and lower water solubility's and are therefore predicted to also have no effects at saturation to aquatic organisms (US EPA 2012).

8.6.1.2 Chronic toxicity endpoints for aquatic organisms

No chronic ecotoxicity data were available for the substance.

8.7 Categorisation and other characteristics of concern

8.7.1 PBT categorisation

The persistence and bioaccumulation of the substance in regards to the domestic hazard criteria is uncertain, although extreme persistence or bioaccumulation is not expected. Further, the substance is not expected to have toxic effects at its limit of solubility. Hence, the substance is not a PBT substance according to domestic environmental hazard criteria.

8.8 Screening assessment

8.8.1 Assessment

The substance is a UVCB that consists of linear and branched alkanes with 12 to 26 carbon atoms. It contains components with no readily dissociable functions and therefore will not ionise in the aquatic compartment. If released to the environment, the substance is expected to partition to the air, soil and sediment and is not expected to cause toxic effects in aquatic organisms due to its limited bioavailability. The substance is not predicted to be persistent in air. In water, soil or sediment the substance is expected to be eventually degraded by biotic and abiotic processes forming water and oxides of carbon.

Release of significant volumes of the substance directly to aquatic ecosystems may cause concerns based on the physical coating of surfaces (for example, bird feathers) and

temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations as the substance is degraded by microorganisms. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate concentrations of the substance in aquatic ecosystems. Spills of larger volumes of the substance are expected to be cleaned up before they can be released to surface waters.

8.9 Outcome

A Tier 1 assessment of the environmental risks from the use of Alkanes, C_{12-26}-branched and linear is not required.

8.10 References

EC and HC 2015a, Final screening assessment, petroleum sector stream approach, fuel oil no. 2, [fuels], chemical abstracts service registry number, 68476-30-2, Environment Canada and Health Canada, viewed 4 September 2015 <http://www.ec.gc.ca/ese-ees/CA593523-4175-4FC0-8546-A8A9482FF242/FSAR_PSSA-S3_FO%20No.%202_EN.pdf>.

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US NLM 2013, Hazardous substances data bank, United States National Library of Medicine, Bethesda, Maryland, USA, viewed 16 September 2014 <http://toxnet.nlm.nih.gov>.

van Leeuwen CJ and Hermens JLM 1995, Risk assessment of chemicals: an introduction, Kluwer Academic Publishers, Dordrecht, The Netherlands.

9 Fatty acid esters

Confidentiality from public disclosure was claimed for the name and Chemical Abstracts Service Registry Number (CAS RN) of this chemical. Information about the chemical subject to commercial-in-confidence claims was provided to the assessment team and a detailed screening assessment of the chemical was conducted. The chemical is referred to as the 'substance' hereafter.

9.1 Background

The substance is an unknown or variable composition, a complex product of a chemical reaction, or a biological material (UVCB) substance. This UVCB is a mixture of organic chemicals. The substance is used in lubricants and greases, as a fuel additive, for coatings and in ink applications (ECHA 2015). One of the components of this UVCB is widely used in cosmetic products (US EPAa). The substance has an identified use as a friction reducer in drilling fluid formulations used in coal seam gas extraction in Australia. There were no identified uses in fracturing or fracturing pre-treatment formulations.

The substance is readily biodegradable in the environment. Releases of large volumes of the substance to natural waterways may disturb the health of aquatic ecosystems through direct and associated indirect physical chemical effects. For example, rapid biodegradation of large quantities of this UVCB in natural waters may decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life (Stringfellow et al. 2014). However, diffuse low level emissions of the substance to soil or water are not expected to pose a concern to the environment.

9.2 Chemical name and identification

CAS Name	**CBI**
CAS RN	**CBI**

9.3 Physico-chemical properties

Property	
Physical form	Liquid (ECHA 2015)
Melting point	-53 to -30°C (ECHA 2015)
Boiling point	302.35-400.01°C (Calculated, US EPA 2011)
Water solubility	4.7 mg/L at 20°C (GSBL 2015)
pKa	Not applicable
Log Kow	6.68-10.61 (Calculated, US EPA 2011)
Vapour pressure	0.000136-0.191 Pa (Calculated, US EPA 2011)

9.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for the substance:

Pre-assessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
Reach (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

9.5 Environmental fate summary

9.5.1 Partitioning

The substance is slightly soluble in water. The component organic chemicals of this UVCB are not expected to dissociate due to a lack of ionisable functionalities. Based on the low measured water solubility (4.7 mg/L), the high predicted octanol-water partition coefficients (log K_{OW} greater than 6.68), and the low estimated vapour pressures (less than 0.2 Pa), the component chemicals are expected to predominately partition to sediment and soil if released to the environment.

9.5.2 Persistence

The substance is readily biodegradable, achieving greater than 65% biodegradation (based on oxygen consumption) in a study conducted according to the standard OECD test guideline 301D (ECHA 2015).

This substance is therefore considered to be not persistent (Not P) in the environment according to domestic hazard criteria (EPHC 2009).

9.5.3 Bioaccumulation

Although the components of this substance are very hydrophobic based on their estimated log K_{OW} values, they are not expected to pose a bioaccumulation concern in the environment. The substance is readily biodegradable and the component chemicals will be susceptible to biotransformation to polar metabolites within organisms.

9.5.4 Transport

The substance is not persistent in the environment and the component chemicals have low volatility and are likely to be both immobile and degradable in soil. This substance is therefore not expected to undergo long-range transport in the environment.

9.6 Environmental effects summary

9.6.1 Critical environmental effects

9.6.1.1 Acute toxicity endpoints for aquatic organisms

The substance is not expected to cause acute toxic effects in aquatic organisms at its limit of solubility. The following representative measured median effective concentration (EC50) and

median lethal concentration (LC50) values for model organisms were identified for the substance:

Taxon	Endpoint	Method
Fish	96 h LC50 > 10 000 mg/L	Experimental *Brachydanio rerio* (ECHA 2015)
Invertebrates	48 h EC50 = 100 mg/L	Experimental *Daphnia magna* (GSBL 2015)
Algae	72 h EC50 > 100 mg/L	Experimental *Scenedesmus subspicatus* (ECHA 2015)

The acute toxicity test results for fish and invertebrates are based on nominal concentrations that greatly exceeded the maximum water solubility limit of the test material, as evidenced by turbidity in the test solutions. However, no mortalities were observed at any tested concentration and at any observation time period. Therefore, the test substance can be considered to be non-toxic to fish and invertebrates at the limit of water solubility.

The algal results are based on concentration of the water accommodated fractions (WAFs), where test media contains only the fraction of multi-component substances that is dissolved and/or present as a stable dispersion or emulsion (OECD 2000). The above results similarly demonstrate that the chemical does not have toxic effects to algae at the limit of water solubility.

9.6.1.2 Chronic toxicity endpoints for aquatic organisms

The following no-observed-effect concentration (NOEC) value for a model organism was identified for the chemical:

Taxon	Endpoint	Method
Invertebrates	21 d NOEC > 1 mg/L	Experimental *Daphnia magna* (ECHA 2015)

Based on the above acute and chronic toxicity study results, the substance is not toxic (Not Toxic) to aquatic life according to domestic toxicity criteria (EPHC 2009).

9.7 Categorisation and other characteristics of concern

9.7.1 PBT categorisation

The chemical is not a PBT substance according to domestic environmental hazard criteria (EPHC 2009).

9.7.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for the chemical.

9.8 Screening assessment

9.8.1 Assessment

The substance is readily biodegradable, not expected to be bioaccumulative, and does not cause acute toxic effects in the aquatic environment at its limit of solubility in water. Release

of significant volumes of this readily biodegradable substance directly to aquatic ecosystems may cause temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations. However, no long-term adverse effects would be expected from uncontained direct releases to water or soil. Furthermore, spills of large volumes of the substance are expected to be cleaned up before it can be released to surface waters.

Diffuse low-level emissions of the substance to soil or water are not expected to pose a concern to the environment based on the low toxicity and the ready biodegradability of the substance.

9.9 Outcome

A Tier 1 assessment of the environmental risks from the use of this chemical is not required.

9.10 References

ECHA 2015, *Registered substances database*, retrieved from <http://echa.europa.eu/information-on-chemicals/registered-substances>.

EPHC 2009, *Environmental risk assessment guidance manual for industrial chemicals*, Environment Protection and Heritage Council, Canberra, retrieved from <http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals>.

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OECD 2000, *Guidance document on aquatic toxicity testing of difficult substances and mixtures*, Organisation for Economic Co-operation and Development, Paris, France.

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10 Nitrogen

10.1 Background

Nitrogen (or nitrogen gas) is an inert diatomic gas that comprises 76% of air by mass (Jones and Atkins 2002). Nitrogen gas is separated from the atmosphere on an industrial scale and is used as an inert gas or foaming agent in a wide range of industries (Kroschwitz 1999). It is reported to be used in the Australian coal seam gas industry within hydraulic fracturing or pre-treatment formulations. Although its function was not specified, internationally this gas is known to be used for fracturing shallow and water sensitive formations that remain self-propped after fracturing (Stringfellow et al. 2014). Additionally, nitrogen gas can be used as a fluid weight reducer and for proppant suspension in fracturing fluids (DoEHP QG 2015).

Nitrogen gas is chemically inert under atmospheric conditions and is not a bioavailable form of nitrogen, except to specific microorganisms involved in biological nitrogen fixation (Wetzel 2001; VanLoon and Duffy 2005). The principal hazard to organisms from nitrogen gas is therefore a physical effect resulting from the displacement of oxygen which may lead to a risk of asphyxiation. This is not considered likely to be a significant risk to the environment from the use of nitrogen gas in coal seam gas applications because in unenclosed systems at atmospheric pressure this gas will immediately partition into the atmosphere where it will be diluted in air, which is predominantly nitrogen gas.

10.2 Chemical name and identification

CAS Name	**Nitrogen**
CAS RN	7727-37-9
AICS name	Nitrogen
Synonyms	Nitrogen gas Dinitrogen
Structural formula	
Molecular formula	N_2
Molecular weight	28.01 g/mol
SMILES	N#N

10.3 Physico-chemical properties

Property	
Physical form (under atmospheric conditions)	Gas
Melting point	-209.86°C (Weast 1976)
Boiling point	-195.8°C (Weast 1976)
Density	1.25 kg/m^3 (0°C, 101 325 Pa (Weast 1976))
Water solubility (mole fraction)	1.183×10^{-5} (298.15K, 101 325 Pa (Battino 1982))
Water solubility (mg/L)	18.4 mg/L (converted from Battino 1982)
pK_a	Not applicable
Log K_{ow}	0.67 (US EPA 2008)
Henry's Law constant	153 846 Pa m^3/mol (converted from Sander 2015)

10.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for nitrogen gas.

10.5 Environmental fate summary

Dinitrogen is an inert gas under normal atmospheric conditions and therefore has a natural tendency to partition and disperse into the air compartment. The very high measured Henry's Law constant (H = 153 846 Pa m^3/mol) indicates that dissolved dinitrogen will partition overwhelming from water or moist soil into the air compartment, where nitrogen gas is the major constituent of the atmosphere.

Dinitrogen has relatively low solubility in water even under saturation conditions (18.4 mg/L). Concentrations of dinitrogen in environmental waters are generally in equilibrium with the atmosphere. However, stratification effects and seasonal changes in dinitrogen consumption and production by the nitrogen cycle in natural water bodies can perturb local dissolved dinitrogen concentrations (Wetzel 2001).

10.6 Environmental effects summary

Nitrogen gas is the dominant constituent of the atmosphere and is also present at or near saturation concentrations in water. Life is naturally adapted to high concentrations of nitrogen gas in the atmosphere and the presence of saturation concentrations of dinitrogen in water. Except for asphyxiation hazards associated with exclusion of oxygen by this inert gas, nitrogen gas is not considered to be hazardous to life.

10.7 Screening assessment

10.7.1 Assessment

Nitrogen gas is the major constituent of the atmosphere. It is an inert non-toxic gas that is ubiquitous in the environment. Life is naturally adapted to the presence of nitrogen gas as

the dominant component of air. No significant additional environmental exposure to nitrogen gas is expected as a result of its use in coal seam gas applications.

10.8 Outcome

A Tier 1 assessment of the environmental risks from the use of nitrogen gas is not required.

10.9 References

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Wetzel, RG 2001, *Limnology: lake and river ecosystems* (3rd edition), Elsevier, San Diego.

11 Bauxite ($Al_2O_3.xH_2O$), sintered

11.1 Background

The chemical under assessment, bauxite ($Al_2O_3.xH_2O$), sintered (sintered bauxite), was incorrectly identified in the industry survey as having Chemical Abstracts Service Registry Number (CAS RN) 1318-16-7. This CAS RN refers to bauxite. The correct CAS RN for sintered bauxite is 144588-68-1. The following assessments refers to this chemical.

Sintered bauxite is a processed form of bauxite, a rock type containing a variety of aluminium hydroxide minerals including gibbsite ($Al(OH)_3$), boehmite (γ-AlO(OH)), and diaspore (α-AlO(OH)), as well as impurities such as silica, iron oxide, and titanium (NSW DPI 2015 and 2008). Aluminium is the most abundant metallic element on the Earth's surface (Geoscience Australia 2012), and bauxite is formed as rocks containing high concentrations of aluminum are leached of almost all other elements over geological timescales. There are large bauxite deposits throughout eastern Australia, with Australia being the largest exporter of bauxite in the world (NSW DPI 2015 and 2008).

Sintered bauxite is made by heating bauxite to remove water (calcination), which will form aluminium oxide (Al_2O_3). The manufacture of sintered bauxite involves mixing finely ground bauxite with binding materials and water, which is shaped into pellets and sintered in a kiln at 1400-1500°C (Mortensen 2007; US ITC 1989). Sintered bauxite is useful as a proppant in the coal seam gas industry because of its high crush resistance, and because the particle size and specific gravity of the beads produced by the sintering process can be tailored to end user requirements (King 2015).

Simple aluminium compounds can be toxic to aquatic organisms if they are made bioavailable through dissolution in the aquatic environment. However, at normal pH, the aluminium compounds expected to be found in sintered bauxite are highly insoluble, and the potential for toxic effects is expected to be low. The solubility of these compounds increases as pH decreases, with maximum toxicity occurring around pH 5.0–5.2. Nevertheless, under acid conditions, the physico-chemical stress to aquatic organisms caused by the low pH is generally of higher concern than low concentrations of dissolved aluminium (ANZECC and ARMCANZ 2000).

11.2 Chemical name and identification

CAS Name	**Bauxite ($Al_2O_3.xH_2O$), sintered**
CAS RN	144588-68-1
AICS name	Not on AICS
Synonyms	Sintered bauxite
Formula	Not available

11.3 Physico-chemical properties

No physico-chemical property data were identified for sintered bauxite. Based on the properties of aluminium oxide, which is the principal component of sintered bauxite, the substance is expected to be a refractory solid, with a melting point greater than 1500°C (LMC 2014).

11.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified in Australia or internationally for sintered bauxite.

11.5 Environmental fate summary

Sintered bauxite is expected to have low solubility under typical environmental conditions. Any small quantities of aluminium ions released to surface water are expected to complex with particulate organic matter and mineral particles and hence predominately partition to the sediment compartment. Similar behaviour is expected if the substance is released to surface soil, where it will not be mobile.

Under acid conditions, there is an increased potential for sintered bauxite to release soluble forms of aluminium to the environment. Many soils in Australia are acidic and contain background levels of naturally occurring aluminium compounds. In these soils, aluminium mobilisation is known to occur, and release of sintered bauxite to these soils has potential to contribute to this phenomenon. Similar behaviours are expected in acid aquatic ecosystems.

11.6 Environmental effects summary

No relevant acute or chronic toxicity data for sintered bauxite were identified.

Under typical environmental conditions, the aluminum ions present in sintered bauxite are not expected to be soluble, and will therefore not be bioavailable to cause toxic effects in aquatic environments. Toxicity in the soil compartment is expected to be similarly limited by low bioavailability.

At low pH levels, soluble forms of aluminium may cause toxic effects. In soils, toxic effects can be observed in plants at concentrations greater than 2 to 5 mg/kg, depending on the plant species (WA Department of Agriculture and Food 2014). In the aquatic environment, toxicity at low pH has been observed in fish (*Salmo trutta*) at 15 µg/L. However, the physico-chemical stress to aquatic organisms caused by the low pH is generally of higher concern than elevated concentrations of dissolved aluminium ions (ANZECC and ARMCANZ 2000).

11.7 Categorisation and other characteristics of concern

11.7.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals including materials such as sintered bauxite according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment and biota (UN ECE 2007; US EPA 2007).

11.7.2 Other characteristics of concern

There are no other characteristics of concern for sintered bauxite.

11.8 Screening assessment

11.8.1 Assessment

Bauxite is a naturally occurring, aluminium-rich rock that is present in many terrestrial and aquatic environments, and is non-toxic under typical environmental conditions. Sintered bauxite, a processed form of bauxite, is expected to have similar environmental characteristics and mainly settle in sediment and soil compartments.

Aluminium compounds are insoluble under typical environmental conditions. Under acidic environmental conditions, bioavailable forms of aluminium can be released and cause toxic effects. However, aluminium is the most abundant metallic element on the Earth's surface, and contributions from the use of sintered bauxite in coal seam gas to any toxicity observed under these conditions are expected to be of low significance.

11.9 Outcome

A Tier 1 assessment of the environmental risks from the use of sintered bauxite is not required.

11.10 References

ANZECC and ARMCANZ 2000, Australia and New Zealand Environment and Conservation Council and Agriculture and Resource Management Council of Australia and New Zealand 2000, Australian and New Zealand Guidelines for Fresh and Marine Water Quality (Vol. 1), Australian Water Association, Artarmon, NSW.

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NSW DPI 2015, Bauxite: Opportunities in NSW. Flyer. NSW Department of Primary Industries, Sydney. Accessed: http://www.resourcesandenergy.nsw.gov.au/__data/assets/pdf_file/0008/545417/bauxite-flyer.pdf

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WA Department of Agriculture and Food 2014, *Effects of soil acidity*, retreieved from <https://www.agric.wa.gov.au/soil-acidity/effects-soil-acidity>.

12 Modified guar gum

12.1 Background

Guar gum is a product obtained from the ground up bean (mainly endosperm) from the guar plant (*Cyamopsis tetragonoloba*). The global guar gum industry is vast with an estimated production in India, the major producer of guar, of 2.7 million tons between 2013 and 2014 (Singh 2014). Most of the demand for the gum is due to the expansion of the shale gas and oil industries with 90% of the export from India used for the extraction of oil and shale gas (Jain 2013; Ministry of Commerce and Industry 2015). Guar gum is used in large volumes by the oil and gas industry in hydraulic fracturing fluids where it functions as a gelling agent (Stringfellow et al. 2014). Other common uses are as an ingredient in ice cream and toothpaste, as a thickener in cosmetics and in the paper industry, and as a component of pesticide product formulations (Singh 2014).

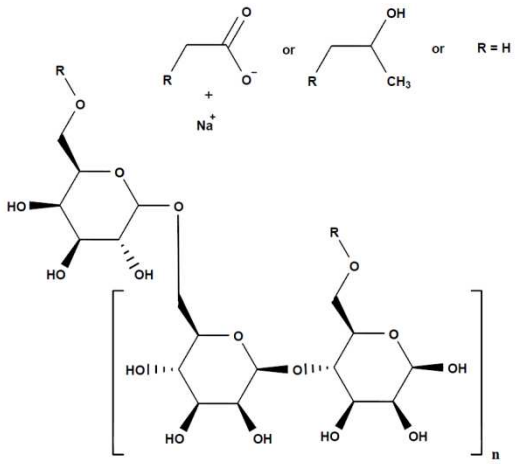
Guar gum is a high molecular weight biopolymer composed of galactomannans. These galactomannans are polysaccharides composed of linear chains of 1,4-linked β-D-mannopyranosyl units with 1,6-linked α-D-galactopyranosyl units as pendant groups attached to the polymannose backbone chain. The ratio of mannose to galactose in galactomannan of guar gum is approximately 2:1, which gives rise to a pendant galactose unit attached to every other mannose unit in the chain
(Joint FAO/WHO Expert Committee on Food Additives 2006; Yoon et al. 2008).

To improve performance and thermal stability for the coal seam gas industry, guar gum is chemically modified with various chemical agents. Guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt (CMHPG sodium salt) is a more stable form of guar gum, that is obtained from the native guar through irreversible nucleophilic substitution involving propylene oxide and chloroacetic acid (Lapasin et al. 1995; Mathur 2012; Pasha and Ngn 2008). It is an anionic modified biopolymer that is used in the oil and coal seam gas industries as a gelling agent for viscosity control. It increases the viscosity of the fracturing fluid to allow more proppant (a material that keeps a fracture open, typically sand) to be carried into the fractures (Commonwealth of Australia 2014; Mathur 2012). Within the Australian coal seam gas industry guar gum and CMHPG sodium salt are specified as being used for hydraulic fracturing or pre-treatment formulations as a gelling agent or clay stabiliser (Commonwealth of Australia 2014; Mathur 2012).

Cross-linkers such as boric acid and various borates are added to fracturing fluids to chemically bind individual CMHPG polymer molecules together to form larger molecules, resulting in higher viscosity, more elasticity, and better proppant transport compared with the polymers without cross-linkages (Stringfellow et al. 2014).

A release of large volumes of modified guar gum into natural waterways may disturb the health of aquatic ecosystems through direct and indirect physical and chemical effects. For example, rapid biodegradation of large quantities of CMHPG sodium salt in natural water bodies could decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life.

12.2 Chemical name and identification

CAS Name	Guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt
CAS RN	68130-15-4
AICS Name	Guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt
Synonyms	CMHPG sodium salt Sodium carboxymethyl hydroxypropyl guar Carboxymethyl hydroxypropyl guar
Structure	
Chemical class	Modified biopolymer
Molecular weight (polymer)	1.9 to 2.2×10^6 g/mol
Sugar monomers	Mannose, Galactose
Degree of Substitution	1.5

12.3 Physico-chemical and biological properties

Carboxymethyl hydroxypropyl guar is a chemically modified linear polysaccharide (galactomannan) with physico-chemical and biological properties similar to those of the parent guar gum (Montgomery 2013; Pasha and Ngn 2008). It is a hydrophilic gelling agent that can be cross-linked through the free hydroxyl units of the pendant α-D-galactopyranosyl residues by different boron and zirconium complexes to high-strength gels (Stringfellow et al. 2014). The viscosity of CMHPG is less affected by temperature, pH and electrolyte concentration and it is also more resistant to hydrolysis compared to the unmodified guar gum (Pasha and Ngn 2008).

CMHPG has a degree of substitution (DS) of 1.5 indicating that on average 1.5 hydroxyl groups are substituted per galactomannan monomer (see structure) (Pasha and Ngn 2008). This places CMHPG in an uncertain category in terms of potential for biodegradation based on DS as for cellulose derivatives, polymers with a DS less than one are more easily degradable than those with a DS greater than two (Simon et al. 1998). However, available information suggests that the modified guar gum polymer can be degraded abiotically including by heat and physical stress (Montgomery 2013; Pasha and Ngn 2008), and through the action of naturally occurring enzymes. According to industry information, the chemically modified guar CMHPG can be enzymatically digested by the same enzymes that also break

down unmodified guar gum (Verenium 2012). A separate study found that closely related modified guars are degraded by the same enzymes that break down unmodified guar gum (Cheng and Prud'homme 2000).

12.4 Domestic and international regulatory information

No specific environmental regulatory controls or concerns were identified within Australia and internationally for guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt.

12.5 Environmental fate summary

Carboxymethyl hydroxypropyl guar is used predominantly in hydraulic fracturing fluids. It is structurally very similar to guar gum, devoid of hazardous functional groups and is susceptible to degradation by enzymes which also degrade natural guar gum (Cheng and Prud'homme 2000; McCleary and Matheson 1983; Verenium 2012). The environmental fate of the modified guar gum is therefore expected to be similar to the fate of its parent biopolymer.

Galactomannans, the sugar polymers of guar gum, can be found in a wide range of plants in the environment and mechanism are in place to degrade them (Buckeridge et al. 2000). When guar gum is released into the environment it will be exposed to β-D-Mannanases, enzymes produced by plants, fungi and bacteria to hydrolyze galactomannans. These enzymes will break down the galactomannans in guar gum to short polysaccharides and their constituent sugars (Buckeridge et al. 2000; Cheng and Prud'homme 2000). Although CMHPG is more stable compared to guar gum (Pasha and Ngn 2008), it is nevertheless expected that the modified guar gum will be degraded in the environment through similar mechanisms as unmodified guar gum. The degradation products of CMHPG can then be further mineralised and/or used by microorganisms as substrate in their anabolic pathways.

Release of CMHPG sodium salt to aquatic ecosystems may cause temporary changes in water quality for local organisms through an increase in biological oxygen demand (BOD) as a result of the microbial degradation of the modified biopolymer. In its application in hydraulic fracturing, the polymer is injected into the coal seam together with proppant and other chemicals such as cross-linkers. It remains there until it is broken down by either enzymes, chemicals or physical stress to lower molecular weight (poly-) saccharides, which are removed in the flow-back water (Commonwealth of Australia 2014). These fragments of CMHPG are potentially more bioavailable and more rapidly digested by microbes, thereby potentially increasing the short-term impacts on dissolved oxygen levels in aquatic ecosystems.

12.6 Environmental effects summary

No evidence of direct ecotoxicological hazards could be identified for CMHPG sodium salt in the scientific literature, reports and patents, at the time of this assessment. Nevertheless, the environmental effects of the modified guar gum are expected to be similar to the effects of its parent biopolymer based on its use, structure, biodegradation profile and lack of hazardous functional groups (Cheng and Prud'homme 2000; Commonwealth of Australia 2014; Cosmetic Ingredient Review 2012; Gangotri et al. 2012; Stringfellow et al. 2014).

One study investigated the potential of guar gum and guar gum derivatives (including CMHPG) as a replacement for agar as a gelling agent in microbial growth media. All fungi and bacteria exhibited normal growth and differentiation on all tested media (Gangotri et al 2012). This indicates that CMHPG does not display acute toxicity to microorganisms.

Guar gum, hydroxypropyl guar and other modified guar gums have reported uses or were investigated for potential uses in the pharmaceutical industry (Swamy 2008). Additionally, modified guar gums are used extensively in the cosmetics industry where they are used at concentrations up to 93% (hydroxypropyl guar in a leave-on hair straightener). The report concluded that the uses of galactomannans are safe in the present practices (Cosmetic Ingredient Review 2012). This is taken to indicate that modified guar gums have limited potential to harm mammals and other terrestrial animals through direct concentrated exposure.

The principal concern for the use of CMHPG sodium salt in hydraulic fracturing is that gelling agents will contribute significantly to the biological oxygen demand (BOD) of flow-back water. Degradable organic gelling agents (such as guar gums and their derivatives) are used in large quantities for hydraulic fracturing operations, which could make implementation of some water treatment processes, such as reverse osmosis (RO), difficult. High concentration of dissolved organic matter may encourage microbial processes that can cause fouling on membrane surfaces used in RO (Stringfellow et al. 2014).

The chemical oxygen demand associated with the microbial oxidation of guars also has the potential to deplete local dissolved oxygen concentrations if CMHPG sodium salt, or its typical degradants, are released directly into the aquatic environment. Consequently, CMHPG sodium salt maybe considered to be capable of causing non-toxic physico-chemical stress to aquatic ecosystem. These effects are considered more likely to be a potential source of environmental harm than any potential ecotoxicity of guars, considering the reported EC_{50} of guar gum for *Daphnia magna* is 42 mg/L (Biesinger et al. 1976).

12.7 Screening assessment

12.7.1 Assessment

CMHPG sodium salt could be released into the environment either as a polymer or, more likely, as its breakdown products such as poly- and mono-saccharides. Closely related galactomannans (i.e. guar gum) are already present in the environment and there are both natural biological and abiotic processes that degrade these biopolymers. It is reasonable to assume that carboxymethyl hydroxypropyl guar will be degraded though the same processes. Additionally, CMHPG sodium salt and closely related polymers have no significant demonstrated acute toxicity. Because of the biodegradability and high molecular weight of guar gum and closely related polymers, no chronic toxic effects are expected.

However, CMHPG sodium salt can be considered as a potential physico-chemical stressor that is non-toxic, but can nevertheless directly or indirectly affect aquatic ecosystems and biota by introducing excessive nutrients to water bodies resulting in temporary oxygen depletion (high BOD). The biological oxygen demand associated with the microbial oxidation of CMHPG should be considered in the treatment of waste water from hydraulic fracturing to avoid any potential adverse effects associated with oxygen depletion in natural waterways.

12.8 Outcome

A Tier 1 assessment of the environmental risks from the use of guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt is not required.

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13 Gelatins

13.1 Background

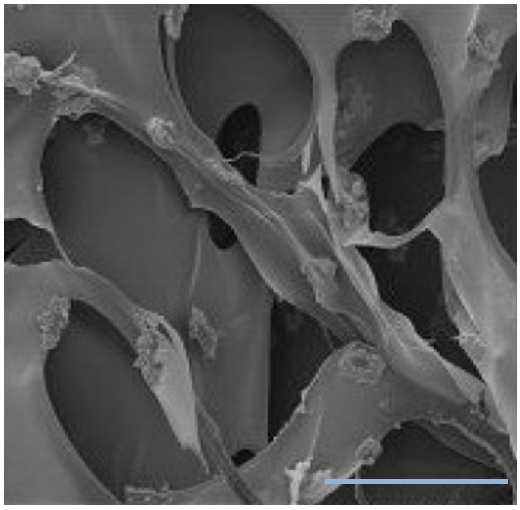
Gelatin is a biopolymer derived from collagen, a naturally occurring protein. Collagen is a polypeptide and the main protein component of the skin, bones and connective tissue of animals, including fish and poultry. It is the single most abundant protein in the animal kingdom and there are at least 28 types of collagen that vary in size and structure (Lodish 2000; Shoulders and Raines 2009). Ninety percent of collagen is made up of three polypeptide chains that form a right-handed triple-helical structure (Hulmes 2008). Gelatin is obtained by acid, alkaline, or enzymatic hydrolysis of collagen's triple-helix organisation at those sites where covalent cross-links join the three peptides. This leads to polydisperse polypeptide mixtures with average molecular weight of 40 to 300 kDa, compared to the ~100 kDa of an individual collagen chain (Gelatine Manufacturers Institute of America 2012; Gorgieva and Kokol 2011; Zhang 2006).

Gelatin as a material does not occur freely in nature but can be considered as hydrolysed and partially degraded collagen instead. There are no plant sources for this polypeptide which is used commercially in numerous industries including pharmaceuticals, food, photography, detergents and hydraulic fracturing in coal seam gas (Committee on Energy and Commerce 2011; Gelatine Manufacturers Institute of America 2012). In the coal seam gas industry, gelatin is used in hydraulic fracturing as an oxygen scavenger/corrosion inhibitor (Government of Western Australia - Department of Mines and Petroleum 2015).

If gelatin is released into the aquatic environment in sufficient quantities it could potentially disturb the health of natural waterways and other aquatic ecosystems through direct and indirect physical and chemical effects. Rapid biodegradation of gelatin in natural water bodies could decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life (Stringfellow et al. 2014). Gelatin is a rich source of amino acids and other nutrients and the sudden increase of nutrients could also cause the rapid growth of microorganism putting further stress on the waterways.

13.2 Chemical name and identification

CAS Name	**Gelatins**
CAS RN	9000-70-8
AICS name	Gelatins
Synonyms	Gelatin Gelatine

CAS Name	Gelatins
3D scanning electron microscopy structure of gelatin (bar is 50µm)[1] [1]Source: (Jeevithan et al. 2014)	
Molecular weight range	40-300 kilodaltons (kDa)
Isoelectric point	pH 4-9
Chemical class	Biopolymer

13.3 Physico-chemical and biological properties

Gelatin is hydrolysed and partially degraded collagen obtained by acid, alkaline, or enzymatic hydrolysis. It is a polypeptide and depending on the source of collagen and the method of its manufacturing process of recovery from collagen, gelatin contains an average of the following amino acids: glycine 21%, proline 12%, hypoproline 12%, glutamic acid 10%, alanine 9%, arginine 8%, aspartic acid 6%, lysine 4%, serine 4%, leucine 3%, valine 2%, phenylalanine 2%, threonine 2%, isoleucine 1%, hydroxylysine 1%, histidine <1% and tyrosine <0.5% (Gorgieva and Kokol 2011).

Depending on the mode of hydrolysis, the isoelectric point of the gelatins range from pH 4 to 9 (See, 2010; Zhang 2006) and the molecular weight ranges from 40 to 300 kDa (Gelatine Manufacturers Institute of America 2012; Gorgieva and Kokol 2011; Zhang 2006). Unlike collagen, gelatin hydrates readily in hot water (but is relatively insoluble in cold water). When added to cold water, gelatin granules swell by absorbing 5 to 10 times their weight in water. Raising the temperature above 40°C dissolves the swollen gelatin particles forming a solution (Gelatine Manufacturers Institute of America 2012; Gorgieva and Kokol 2011; Northrop 1926).

Gelatin can undergo reversible solution-gel transformation (sol-gel) and forms a gel when cooled down to the gelling point by reforming gelatin chains (Djabourov 1988; Gorgieva and Kokol 2011). The actual nature of the 3D network of gelatin is not well defined, localised ordered regions interconnected with amorphous regions of randomly coiled segments have been proposed in the literature (Peña et al. 2010).

13.4 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for gelatin.

13.5 Environmental fate summary

Within the context of potential releases of gelatin into the environment as a result of its use in coal seam gas extraction, the fate of the biopolymer is predicted to be regulated by abiotic and biotic breakdown.

Unlike its parent biopolymer collagen, which is insoluble and only degradable by specific enzymes (Etherington 1977; Shoulders and Raines 2009), gelatin hydrates readily in water and is susceptible to degradation by most proteases (Gorgieva and Kokol 2011). Gelatin, as a protein, is subject to rapid biodegradation when the environmental conditions are adequate (Abrusci et al. 2004). The issue of biodegradation by microorganism is of such importance to the gelatin industry that the production facilities are routinely monitored for bacterial contamination. Ultra-high temperature treatment (UHT) of gelatin is employed to minimise the potential for contamination with microorganism (De Clerck et al. 2004). Even after UHT, members of the genus *Bacillus*, *Salmonella*, *Kluyvera*, *Staphylococcus*, *Burkholderia*, *Enterococcus*, *Pseudomonas*, *Yersinia*, *Streptococcus* and *Brevundimonas* were detected in a study of bacterial contamination of gelatin (De Clerck et al. 2004).

When investigating the gelatin digesting potential of various bacteria derived from cinematographic films, biodegradation of photographic grade gelatin was detected in 50% of the strains under various conditions (Abrusci et al. 2004). Most of the bacteria found colonising these films were resistant to adverse environmental conditions (Abrusci et al. 2007). The natural mixture of Bacillus (*B. amyloliquefaciens* and *B. subtilis*) present in the photographic films showed a synergistic effect in the biodegradation of gelatins (Abrusci et al. 2004). Next to bacteria, fungi were also identified to degrade gelatin under various conditions (Abrusci et al. 2007). Both, bacteria and fungi, release reactive oxygen species (ROS) when digesting gelatin at lower temperatures, further oxidising and degrading the biopolymer (Abrusci et al. 2007).

Based on this information, any gelatin released into aquatic ecosystems will be rapidly degraded by microorganisms through enzymatic digestion to the individual amino acids or short peptides. If sufficient quantities of gelatin were abruptly released into a water body, this could cause temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations.

13.6 Environmental effects summary

Based on the biological properties and the environmental fate of gelatin, especially the rapid biodegradation, prolonged exposure of aquatic organisms to the biopolymer will be highly unlikely (Abrusci et al. 2004; Abrusci et al. 2007; De Clerck et al. 2004).

To investigate the potential of acute toxicity of gelatin, dogs were injected intravenously with high concentration of the polypeptide. Administration of gelatin by vein for two to three days (a total of 1 to 3 g/kg) did not show adverse effects in dogs indicating that gelatin does not have acute toxicity (Robscheit-Robbins et al. 1944).

Gelatin as a rapidly biodegradable protein is a rich source of amino acids and other nutrients such as nitrogen and carbon for bacteria and fungi. The increased bioavailability of nutrients could lead to a significant increase in biological oxygen demand (BOD) as a result of degradation of gelatin and the stimulated growth of microorganisms (Koser et al. 1938). High BOD will deplete local dissolved oxygen concentrations when gelatin or its breakdown products are released into the aquatic environment in sufficient quantities relative to the volume of the receiving water body. This depletion of oxygen has the potential to place significant stress on some organisms within the aquatic environment.

13.7 Screening assessment

13.7.1 Assessment

Gelatin could be released into the environment either as a polymer or as breakdown products such as polypeptides and amino acids. Gelatin is biodegradable by many naturally occurring enzymes and there are abiotic processes that also degrade this biopolymer. As experiments in dogs demonstrated, acute toxicity of gelatin is not expected and because of its biodegradability chronic toxic effects are also highly unlikely.

Gelatin can best be described as a potential physico-chemical stressor that is non-toxic but can nevertheless directly affect ecosystems and biota by adding excessive nutrients to water bodies resulting in oxygen depletion (high BOD).

Based on the relatively rapid biodegradation and expected low aquatic toxicity of gelatin and its likely degradants, use of this substance in coal seam gas extraction is unlikely to result in direct toxic effects on the environment. However, the biological oxygen demand associated with the breakdown of gelatin should be considered in the treatment of waste water to avoid adverse effects associated with oxygen depletion in environmental waters if they receive treated waste water from coal seam gas production sites.

13.8 Outcome

A Tier 1 assessment of the environmental risks from the use of gelatin is not required.

13.9 References

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14 Group assessment – Simple inorganic salts

10377-60-3 Nitric acid, magnesium salt
7727-43-7 Sulfuric acid, barium salt (1:1)
7772-98-7 Thiosulfuric acid ($H_2S_2O_3$), disodium salt

14.1 Grouping rationale

This group contains three simple inorganic salts. The members of this group have each been assessed based on their respective potential to dissolve and dissociate into their constituent cations and anions, and the likely impacts of the released ions under typical environmental conditions.

14.2 Background

The simple inorganic salts assessed within this report have a wide range of commercial and industrial uses. Magnesium nitrate (CAS RN: 10377-60-3) has significant use as a chemical intermediate in the production of a range of products, including fertilisers. Barium sulfate (CAS RN: 7727-43-7) is used extensively in drilling fluids, but also as a pigment or filler in paper, plastics, paints and cosmetics. It is also known for its use as a contrast agent for X-ray procedures. Sodium thiosulfate (CAS RN: 7772-98-7) is used for bleaching pulp during paper manufacture, as a mordant for dyes, and to neutralise chlorine (ECHA 2015; HSDB, 2015).

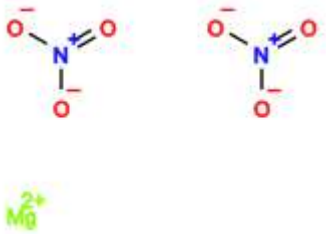
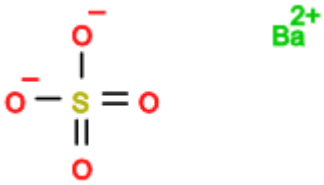
In the coal seam gas industry, magnesium nitrate is used for microbial control during hydraulic fracturing or in fracturing pre-treatment formulations, as well as for clay management (DoEHP QG 2015). Barium sulfate is reported to be used as a weighting aid in drilling fluid formulations, while sodium thiosulfate is reported to be used as a chlorine neutraliser/gel stabiliser in hydraulic fracturing or pre-treatment formulations.

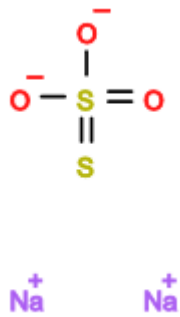
Under typical environmental conditions, magnesium nitrate and sodium thiosulfate are expected to dissolve in water and fully dissociate into nitrate and magnesium ions, and thiosulfate and sodium ions, respectively. These ions have a number of important functions in the environment. Magnesium and sodium ions are ubiquitous in the environment and are essential for proper functioning of cells (Campbell et al. 1999). Nitrates form a pivotal part the global nitrogen cycle, and are an essential plant nutrient (Barsanti and Gualtieri 2010). Thiosulfate is an important component of the global sulfur cycle (Jørgensen 1990).

If released in high volumes, however, these ions could potentially cause physico-chemical stresses in aquatic environments by direct and indirect pathways. For example, release of large amounts of these soluble salts directly into waterways has the potential to directly cause adverse effects on aquatic life by increasing the salinity of the water body (ANZECC and ARMCANZ 2000). Direct and indirect stress could also occur as the result of excessive levels of nitrate which can cause eutrophication. Eutrophication can lead to a decrease in dissolved oxygen to levels which are insufficient to sustain normal respiration by aquatic life (VanLoon and Duffy 2005; AWWA 2006). Thiosulfate ions have some potential to reduce the reduction-oxidation potential of some aquatic ecosystems (Cotton and Wilkinson 1988). However, numerous natural biogeochemical mechanisms exist which tend to limit fluctuations in nutrient levels, which occur frequently in healthy aquatic ecosystems.

Barium sulfate has low solubility in water with a solubility product (K_{sp}) of 1.1×10^{-10} (Reger et al. 2009). Under typical environmental conditions, barium sulfate will undergo limited dissolution and dissociation into its constituent ions. Therefore, although barium ions can cause toxic effects, environmental release of barium sulfate is not expected to result in significant release of ionic barium in a bioavailable form (ATSDR 2002; Menzie et al. 2008; Selinger 1988).

14.3 Chemical name and identification

CAS Name	**Nitric acid, magnesium salt (2:1)**
CAS RN	10377-60-3
AICS name	Nitric acid, magnesium salt
Synonyms	Magnesium nitrate
Structural formula	
Molecular formula	$Mg(NO_3)_2$
Molecular weight	148.31 g/mol
SMILES	[Mg++].[N+](=O)([O-])([O-]).[N+](=O)([O-])([O-])
CAS Name	**Sulfuric acid, barium salt (1:1)**
CAS RN	7727-43-7
AICS name	Sulfuric acid, barium salt (1:1)
Synonyms	Barium sulfate Barite
Structural formula	
Molecular formula	$BaSO_4$
Molecular weight	233.39 g/mol
SMILES	S(=O)(=O)([O-])([O-]).[Ba++]
CAS Name	**Thiosulfuric acid ($H_2S_2O_3$), sodium salt (1:2)**
CAS RN	7772-98-7
AICS name	Thiosulfuric acid ($H_2S_2O_3$), disodium salt

CAS Name	**Nitric acid, magnesium salt (2:1)**
Synonyms	Sodium thiosulfate
Structural formula	
Molecular formula	$Na_2S_2O_3$
Molecular weight	158.11 g/mol
SMILES	[Na+].[Na+].S(=S)(=O)([O-])([O-])

14.4 Physico-chemical properties

Property	**Nitric acid, magnesium salt**
Physical form	Solid (ECHA 2015)
Melting point	330°C (dec.) (ECHA, 2105)
Boiling point	Not applicable due to decomposition on heating
Water solubility	712 g/L (ECHA 2015)
Vapour pressure	Not expected to be volatile
Property	**Sulfuric acid, barium salt (1:1)**
Physical form	Solid (ECHA 2015)
Melting point	1580°C (dec.) (ECHA 2015)
Boiling point	Not applicable due to decomposition on heating
Density	4.49 g/cm^3 (HSDB, 2015)
Water solubility	3.1 mg/L (ECHA 2015)
Vapour pressure	Not expected to be volatile
Property	**Thiosulfuric acid ($H_2S_2O_3$), disodium salt**
Physical form	Solid (ECHA 2015)
Melting point	100°C (ECHA 2015)
Boiling point	Not applicable due to decomposition on heating
Water solubility	764 g/L (ECHA 2015)
Vapour pressure	Not expected to be volatile

14.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No relevant environmental regulatory controls or concerns were identified within Australia and internationally for the substances in this group.

14.6 Environmental fate summary

Magnesium nitrate and sodium thiosulfate are readily soluble in water, and are expected to dissociate in the environment to form nitrate and magnesium ions, and thiosulfate and sodium ions, respectively (e.g. Brady and Holum 1984). These ions are naturally ubiquitous substances that are present in all environmental compartments and subject to environmental transport processes (e.g. Campbell et al. 1999; VanLoon and Duffy 2005; Wetzel 2001). As a result, these substances are expected to move to soil, sediment or water compartments upon release.

Nitrate and thiosulfate ions are also expected to undergo biotransformation reactions in the environment. Nitrate ions are a pivotal component of the global nitrogen cycle, and are taken up by plants as nutrients and converted to organic nitrogen compounds (Barsanti and Gualtieri 2010). The thiosulfate ion is a sulfur (VI) oxyanion which goes on to form sulfate (SO_4^{2-}), sulfite (SO_3^{2-}), and dihydrogen sulfide in aquatic environments. These chemicals are formed concurrently through oxidation, reduction, and disproportionation reactions, with the proportions produced depending on whether oxidising or reducing conditions prevail (Jørgensen 1990).

Barium sulfate is the salt of a strong acid and will dissociate in water to barium cations and sulfate anions. However, this salt has only slight solubility in water, and significant dissolution is not expected to occur. Nevertheless, depending on environmental conditions, some release of barium and sulfate ions may occur. Free barium ions are rare in typical aquatic ecosystems, and instead generally precipitate with present sulfate or carbonate ions (ATSDR 2002; Menzie et al. 2008; Selinger 1988). Free sulfate ions are expected to undergo processes similar to those outlined above for the thiosulfate ion.

14.7 Environmental effects summary

A range of ecotoxicity data is available for the chemicals in this group, as well as similar inorganic salts, to demonstrate low toxicity to aquatic organisms. Toxicity endpoints identified generally greatly exceeded 100 mg/L, indicating very low toxicity (ECHA 2015; LMC 2014).

14.8 Categorisation and other characteristics of concern

14.8.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment (UNECE 2007; US EPA 2007).

14.8.2 Other characteristics of concern

No other characteristics of concern were identified for the chemicals in this group.

14.9 Screening assessment

14.9.1 Assessment

The chemicals in this group are simple salts composed of ions that in most cases perform essential roles in environmental systems. Dissolution of magnesium nitrate and sodium thiosulfate is expected to result in the release of their associated ions. Magnesium and sodium ions are ubiquitous in the environment and are essential for proper functioning of cells, while nitrates and thiosulfates form important components of the global nitrogen and sulfur cycles, respectively. Barium sulfate is a common precipitate in environmental waters. In the environment, these chemicals are expected to typically have very low toxicity (or low bioavailability in the case of barium sulfate) and undergo natural transformation and transport process.

Release of significant volumes of the chemicals in this group to aquatic ecosystems may cause temporary changes in water quality for local organisms, such as increased salinity or reduced dissolved oxygen concentrations. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate fluctuations in the concentrations of the ions released from these chemicals in aquatic ecosystems. Spills of larger volumes of the chemicals in this group are expected to be cleaned up before extensive release to surface waters can occur.

14.10 Outcome

A Tier 1 assessment of the environmental risks from the use of the chemicals in the Simple inorganic salts group is not required.

14.11 References

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15 Group assessment – Soluble carbonates

124-38-9 Carbon dioxide
463-79-6 Carbonic acid
584-08-7 Carbonic acid, dipotassium salt
533-96-0 Carbonic acid, sodium salt (2:3)

15.1 Grouping rationale

Carbonic acid and the two salts in this group may be considered as all being derived from the dissolution and hydration of carbon dioxide in water. All four substances are interrelated by common biogeochemical transformation processes, which are ubiquitous in the natural environment. The environmental fate and effects of all four substances have commonalities which are linked by these biogeochemical processes and they have therefore been assessed as a group.

15.2 Background

Carbon dioxide is used in gas and solution form across a wide range of industries including food and beverages, electronics, treatment of drinking water, healthcare and in the production of chemicals (IPCC 2005). Carbonic acid is used in some of the same applications as it is produced when CO_2 dissolves and fully hydrates in water. In gas form, CO_2 is used in many consumer products that require pressurised gas as it is relatively inert. Carbonic acid, sodium salt (sodium sesquicarbonate) also has multiple applications, such as its use in swimming pools, within the paper and pulp industry, as a food additive and pesticide, and in the production of glass, soaps and washing powders (DoEHP QG 2015; OECD 2002; US EPA 2006b). Similarly, carbonic acid, dipotassium salt (potassium carbonate) is used for soap, glass, and china production (DoEHP QG 2015).

Carbon dioxide can be used as a component of coal seam gas fracturing fluids in shallow formations to form a foam (Stringfellow et al. 2014). This reduces the volume required to transport the same amount of proppant (US EPA 2004). Carbonic acid is used as a buffer, stabiliser, and solvent within the coal seam gas industry (DoEHP QG 2015). According to information provided by industry, potassium carbonate is used as a pH buffer in fracturing or fracturing pre-treatment formulations. Sodium sesquicarbonate is reported to be used as a cross-linker, pH buffer, breaker, surfactant, and clay stabiliser in hydraulic fracturing and pre-treatment formulations.

Carbon dioxide is essential for life on Earth and is a respiration product of all aerobic organisms. The concentration of carbon dioxide in the atmosphere, the terrestrial biosphere and the oceans is maintained by the carbon cycle. The carbon cycle is the process that describes the continual exchange of carbon between these environmental compartments. Carbon dioxide is an important atmospheric gas and is released naturally into the atmosphere through the decay and/or combustion of organic matter, respiration, or volcanic activity (Wetzel 2001).

Sodium and potassium carbonate are highly soluble, dissociating into sodium, and/or potassium and CO_3^{2-} in water. Sodium, potassium and carbonate ions occur naturally in the environment and their distribution is widespread (Wetzel 2001). Sodium carbonic acid salts are considered to present no ecotoxicological risk (US EPA 2006). For potassium ions,

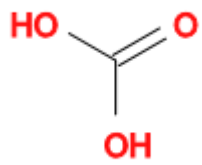
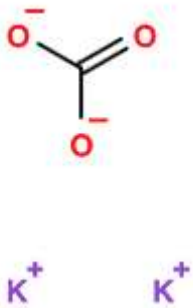
limited data are available for both background concentrations and ecotoxicological activity, however, the risk to terrestrial and aquatic organisms from typical concentrations can be considered low.

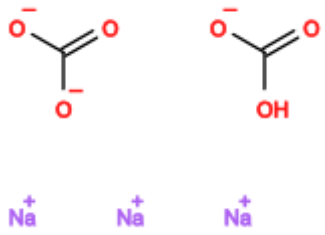
Although the carbonic substances in this group are not considered toxic, excess releases to aquatic systems has the potential to substantially alter pH and salinity. Therefore, this assessment will focus on the potential physico-chemical hazards of these substances to aquatic ecosystems.

15.3 Chemical name and identification

The substance identified as carbonic acid with CAS RN 463-79-6 is not prepared or used as a discrete chemical for industrial purposes. It is the product of the complete hydration of carbon dioxide gas dissolved in water ($CO_{2(g)}$). References to carbonic acid for industrial purposes are therefore taken to indicate an equilibrium solution of dissolved carbon dioxide in water containing some concentration of carbonic acid (H_2CO_3).

CAS Name	**Carbon dioxide**
CAS RN	124-38-9
AICS name	Carbon dioxide
Synonyms	Not applicable
Structural formula	
Molecular formula	CO_2
Molecular weight	44.01 g/mol
SMILES	C(=O)(=O)
CAS Name	**Carbonic acid**
CAS RN	463-79-6
AICS name	Not on AICS
Synonyms	Not applicable

CAS Name	**Carbon dioxide**
Structural formula	
Molecular formula	H_2CO_3
Molecular weight	62.02 g/mol
SMILES	C(=O)(O)(O)
CAS Name	**Carbonic acid, potassium salt (1:2)**
CAS RN	584-08-7
AICS name	Carbonic acid, dipotassium salt
Synonyms	Potassium carbonate Potash
Structural formula	
Molecular formula	K_2CO_3
Molecular weight	138.21 g/mol
SMILES	[K+].[K+].C(=O)([O-])([O-])
CAS Name	**Carbonic acid, sodium salt (2:3)**
CAS RN	533-96-0
AICS name	Carbonic acid, sodium salt (2:3)
Synonyms	Sodium sesquicarbonate

CAS Name	Carbon dioxide
Structural formula	
Molecular formula	$Na_3H(CO_3)_2$
Molecular weight	190.00 g/mol
SMILES	[Na+].[Na+].[Na+].C(=O)([O-])([O-]).C(=O)([O-])(O)

15.4 Physico-chemical properties

Properties	Carbon dioxide (CO_2)	Carbonic acid, dipotassium salt	Carbonic acid, sodium salt (2:3)
Physical form (under atmospheric conditions)	Colourless gas	Colourless crystalline solid	Colourless crystalline solid
Boiling point	-78.5°C (sublimation)	Not available	Not available
Water solubility	1.453 g/L (25°C, 101 325 Pa) (converted from Dean 1999)	1120 g/L (20°C) (Weast 1976)	130 g/L (Weast 1976)
pK_a	pK_a = 6.43	pK_a =10.43 (HCO_3^-) (Wetzel 2001)	pK_a =10.43 (HCO_3^-) (Wetzel 2001)
Henry's Law constant	3000 Pa m^3/mol (converted from Sander 2015)	Not applicable	Not applicable

Carbon dioxide is a water soluble acidic oxide that is slow to reach equilibrium with its hydration products H_2CO_3, HCO_3^- and CO_3^{2-}. The rate determining step is the hydration of $CO_{2(aq)}$ to form H_2CO_3. Conversely, the dissociation of H_2CO_3 is very rapid. In organisms, the hydration reaction is catalysed by the enzyme carbonic anhydrase (Cotton and Wilkinson 1988). For further discussion, see Section 1.6.2.

15.5 Domestic and international regulatory information

Carbon dioxide is a greenhouse gas that is listed under Annex A of the Kyoto protocol (UN 1998).

No other environmental regulatory controls or concerns were identified within Australia or internationally for the substances in the Soluble carbonates group.

15.6 Environmental fate summary

Carbon dioxide and H_2CO_3 are ubiquitous in the environment and are present in all aquatic and terrestrial plants and animals. Carbonate and HCO_3^- ions will readily react with calcium and magnesium to form relatively insoluble carbonate minerals such as calcite and dolomite, leaving sodium and potassium salts dissolved in the water (e.g. Eugster and Jones 1979). Sodium and potassium are nutrients that are regulated through a range of biogeochemical cycles (e.g. Wetzel 2001).

15.6.1 Dissolution and partitioning

Carbon dioxide is very soluble in water (1.453 g/L at 25°C under 1 atm of CO_2). When used in coal seam gas applications, the concentration of CO_2 in water could be significantly higher than this value. However, when released to the environment, CO_2 is expected to rapidly re-equilibrate and partition to the atmosphere. In addition, the speciation of dissolved CO_2 can be affected by other factors as discussed below.

Carbon dioxide is a minor component of the atmosphere, contributing <0.05% to the total volume (Wetzel 2001). Carbon dioxide partitions between the atmosphere and water in proportions given by Henry's Law, where the amount dissolved in water from atmospheric CO_2 is approximately 0.4 mg/L (at 30°C) (Wetzel 2001). However, the concentration of CO_2 in most lakes has been shown to be significantly greater – up to 57 times greater – than the equilibrium concentration (Cole 1994).

Carbon dioxide is continually exchanged between the atmosphere, aquatic systems and terrestrial environments. The carbon cycle naturally regulates the concentration of CO_2 in each environmental compartment by a number of processes including photosynthesis, respiration and weathering. In fresh water, the majority of carbon exists as equilibrium products of carbonic acid. In freshwaters, if CO_2 concentrations are greater than equilibrium values, CO_2 will be lost rapidly to the atmosphere (Wetzel 2001).

Both potassium carbonate and sodium sesquicarbonate immediately dissolve into sodium, potassium, and HCO_3^- ions in aquatic and terrestrial environments upon contact with water (Wetzel 2001).

15.6.2 Speciation

Carbon dioxide is a water soluble acidic oxide. Its speciation reactions in water are as follows:

$$CO_{2(g)} \rightleftharpoons CO_{2(aq)}$$

$$CO_{2(aq)} \rightleftharpoons H_2CO_{3(aq)} \qquad K = 600 \text{ (Cotton and Wilkinson 1988)}$$

$$H_2CO_{3(aq)} \rightleftharpoons H^+_{(aq)} + HCO_3^-{}_{(aq)} \qquad pKa = 3.8 \text{ (Cotton and Wilkinson 1988)}$$

$$HCO_3^-{}_{(aq)} \rightleftharpoons H^+_{(aq)} + CO_3^{2-}{}_{(aq)} \qquad pKa = 10.3 \text{ (Wetzel 2001)}$$

The relative proportion of each inorganic carbon species will be controlled by the pH and ionic strength of the water. Below pH 5, free CO_2 predominates, while above pH 9.5, CO_3^{2-} is the dominant species. Between pH 7 and 9, the concentration of HCO_3^- will be significant. Speciation will also be affected by other properties of the water body including the concentration of other ions such as calcium and iron.

At equilibrium, the concentration of $CO_{2(aq)}$ is significantly larger [by a factor of ~600 (Cotton and Wilkinson 1988)] than that of H_2CO_3. Aqueous CO_2 and H_2CO_3 are commonly treated as a single species, with an apparent pK_a of 6.3, as reported in the above table (Section 1.3). H_2CO_3 itself is significantly more acidic with a pK_a of 3.8.

Salts of H_2CO_3 occur naturally and are commonly found in soil and water (US EPA 2006). Carbonic acid and its salts dissociate rapidly in the environment to establish equilibria with bicarbonate and carbonate ions (HCO_3^- and CO_3^{2-}, respectively). Carbon dioxide can be considered as the parent compound in these complex equilibrium reactions.

15.6.3 Bioaccumulation

Carbon dioxide is essential for life and the regulation of its concentration both in the environment and in organisms is controlled by a number complex processes. In the environment, the carbon cycle regulates CO_2 concentrations and in organisms, enzymatic processes regulate CO_2 concentrations in order to maintain homeostasis.

15.6.4 Transport

Natural processes such as photosynthesis, weathering and respirations regulate the movement of carbon between the atmosphere, oceans, and terrestrial systems. In these systems CO_2 is both produced and absorbed by microorganisms, plants and animals (US EPA 2004).

15.7 Environmental effects summary

Soluble inorganic carbon in the form of carbonates is ubiquitous in the environment. It is essential for life and also forms part of the essential buffering capacity in natural waterways. It is not possible to evaluate the acute and/or chronic effects of soluble inorganic carbon using usual ecotoxicological test methods as it forms part of the buffering test solution.

During the use of CO_2 in coal seam gas applications, additional inputs of CO_2 into waterways (i.e. following a spill) may temporarily perturb the pH of the water. However, this perturbation will be compensated by normal control mechanisms.

15.8 Categorisation and other characteristics of concern

15.8.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment (UNECE 2007; US EPA 2007).

15.8.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for the chemicals in this group.

15.9 Screening assessment

15.9.1 Assessment

Substances in the Soluble carbonates group are essential nutrients in soils and waters, with their concentrations regulated by both biotic and abiotic processes. As such, chemicals in this group are not considered to represent ecotoxicological hazards to the aquatic or soil environment.

In aquatic systems, if the concentration of dissolved CO_2 increases dramatically, the pH of the water can change. This will occur if the equilibrium of total inorganic carbon is disrupted (Wetzel 2001). Following a large spill of carbonic acid into a stream, the pH of the water may decrease outside of the normal pH range tolerated by aquatic organisms. In this manner, substances in the Soluble carbonates group can act as direct physico-chemical stressors as they may perturb pH outside of the normal range. Changes in pH have the potential to affect the mobility of other nutrients and/or toxic chemicals. However, such changes are expected to be short-lived given that high concentrations of carbon dioxide above equilibrium values are lost rapidly to the atmosphere (Wetzel 2001). Inorganic carbon will be re-equilibrated by the natural flux of CO_2 between aquatic systems and the atmosphere.

15.10 Outcome

A Tier 1 assessment of the environmental risks from the use of substances in the Soluble carbonates group is not required.

15.11 References

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16 Group assessment – Limestone and its derivatives

1317-65-3 Limestone
1305-78-8 Calcium oxide

16.1 Grouping rationale

Limestone and calcium oxide were grouped together for the purposes of this report on the basis of their use and chemical behaviour in the environment. Calcium oxide is produced on a very large scale industrially from limestone, and is converted to calcium hydroxide and then calcium carbonate, the major constituent of limestone, under environmental conditions.

16.2 Background

Limestone is the name given to a type of rock mostly composed of calcium carbonate. It also contains minor impurities of iron, magnesium, quartz, clay, pyrite, phosphate, and organic matter (Pohl 2011). It is used widely in agriculture to increase calcium concentrations and the pH of soils (Upjohn et al. 2005). Limestone is used industrially on a very large scale as an ingredient in concrete production and in metallurgy (Oates 1998; Pohl 2011). In the Australian coal seam gas industry, it is used as a bridging agent in drilling fluid formulations.

Calcium oxide is made by heating calcium carbonate, often in the form of limestone, to approximately 900°C to release carbon dioxide (Oates 1998; Pohl 2011). It is a key ingredient in concrete, and is also used for water treatment and paper and pulp production (USGS 2015). Within the Australian coal seam gas industry, calcium oxide is used for pH control in hydraulic fracturing or fracturing pre-treatment formulations.

The behaviour of these chemicals in the environment is initially distinct, but common products are eventually formed. Limestone dissolves slowly in water, releasing calcium and carbonate ions as well as other trace elements (Deer et al. 1992; Clair and Hindar 2005). Conversely, calcium oxide is highly basic when dissolved and reacts immediately with water to form calcium hydroxide (Clair and Hindar 2005). However, this initial hydrolysis product then undergoes further reactions to form calcium carbonate. Calcium and carbonate ions are naturally occurring components of aquatic and terrestrial environments, and generally have low ecotoxicity.

Calcium oxide is a strong base which has the potential to alter the pH of a receiving water body thus causing direct and indirect physico-chemical stress in aquatic ecosystems. However, this base will be rapidly neutralised by reactions with dissolved carbon dioxide and other natural acids in aquatic ecosystems. The products of these neutralisation reactions (e.g. calcium and carbonates ions) are nutrients in aquatic systems and not considered to be toxic to aquatic organisms. These neutralisation reactions are key components of natural biogeochemical mechanisms which tend to limit fluctuations in the pH of healthy aquatic ecosystems.

16.3 Chemical name and identification

Chemical Identity	**Limestone**
CAS RN	1317-65-3
AICS name	Limestone
Synonyms	Not available
Formula	Not applicable
Chemical Identity	**Calcium oxide (CaO)**
CAS RN	1305-78-8
AICS name	Calcium oxide
Synonyms	Quicklime
Formula	CaO
Formula weight	56.08 g/mol

16.4 Physico-chemical properties

Property	**Limestone**
Physical form	Solid
Melting point	Approximately 900°C (dec.) (Oates 1998).
Density	Not available
Water solubility	Not available
Property	**Calcium oxide**
Physical form	Hygroscopic solid
Melting point	2570°C (LMC 2014)
Boiling point	2850°C (LMC 2014)
Water solubility	Reacts with water to form calcium hydroxide
pK_a	12.5 (LMC 2014)

16.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific domestic or international environmental regulatory controls or concerns were identified for limestone or calcium oxide.

16.6 Environmental fate summary

Limestone dissolves slowly in water, releasing calcium and carbonate ions as well as other trace elements, such as iron and magnesium (Deer et al. 1992; Clair and Hindar 2005; Pohl 2011). These trace elements are naturally ubiquitous in the environment and are subject to natural biogeochemical processes. Calcium oxide reacts immediately upon

exposure to water, forming calcium hydroxide, which itself reacts with carbon dioxide to form calcium carbonate. The final reaction products of both limestone and calcium oxide in the environment are therefore essentially the same, although calcium oxide typically has lower concentrations of magnesium and other inorganic chemicals than limestone and produces a higher initial concentration of hydroxide ions (Upjohn et al. 2005).

Calcium and carbonate ions occur naturally in all environmental compartments, and are important nutrients for various organisms. Calcium is mobile in soil (ANZECC and ARMCANZ 2000) and, if released to the environment, should be expected to experience significant partitioning to the water compartment. However, calcium ions may also form insoluble precipitates with anions present in the environment, such as carbonate ions, and settle out of the aqueous phase. Carbonate is an important component of the global carbon cycle (Wetzel 2001).

16.7 Environmental effects summary

Calcium carbonate has low toxicity to aquatic and terrestrial organisms. Ecotoxicological endpoint values for aquatic organisms generally greatly exceed 100 mg/L (LMC 2014), indicating very low toxicity.

16.8 Categorisation and other characteristics of concern

16.8.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals including limestone and calcium oxide according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment (UNECE 2007; US EPA 2007).

16.8.2 Other characteristics of concern

There are no other characteristics of concern for limestone or calcium oxide.

16.9 Screening assessment

16.9.1 Assessment

The two chemicals in this group are expected to predominantly release calcium and carbonate ions to the environment. These ions are naturally ubiquitous in all environmental compartments and are essential to life in various organisms. They are expected to have very low toxicity and undergo natural transformation and transport processes.

Release of significant volumes of the chemicals in this group directly to surface waters may cause temporary changes in water quality for local organisms, such as pH changes. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate changes in pH. Spills of larger volumes of these chemicals are expected to be cleaned up before they can be released to surface waters.

16.10 Outcome

A Tier 1 assessment of the environmental risks from the use of substances in the Limestone and its derivatives group is not required.

16.11 References

ANZECC and ARMCANZ 2000, Australia and New Zealand Environment and Conservation Council and Agriculture and Resource Management Council of Australia and New Zealand 2000, Australian and New Zealand Guidelines for Fresh and Marine Water Quality (Vol. 1), Australian Water Association, Artarmon, NSW.

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Wetzel, RG 2001, *Limnology: lake and river ecosystems* (3rd ed.), Elsevier, San Diego.

17 Group assessment – Silica

7631-86-9 Silica
112926-00-8 Silica gel, precipitated, crystalline free
91053-39-3 Kieselguhr, calcined
14808-60-7 Quartz (SiO_2)
14464-46-1 Cristobalite (SiO_2)
15468-32-3 Crystalline silica, tridymite

17.1 Grouping rationale

This group comprises six inorganic substances which are predominantly composed of silica (SiO_2). The group includes both amorphous and crystalline forms of silica. All six substances have been assessed as a group because they share similar physical and chemical characteristics, and they are all expected to share a similar fate if released into the environment.

17.2 Background

Silica, also known as silicon dioxide, occurs naturally in vast quantities on the surface of the Earth. Crystalline mineral forms of silica (such as quartz) are important constituents of most igneous, metamorphic and sedimentary rocks. Silica (in the form of quartz) also occurs as a secondary mineral in veins formed as silica precipitates from hydrothermal groundwater as it cools (Deer et al. 1992). Silica is present in most soils in one or more forms (CSIRO Division of Soils 1983; Jones and Atkins 2002; Wetzel 2001).

Silica takes many forms, which can be categorised as either crystalline or amorphous based on the presence or absence of long-range order in the structure. This group comprises amorphous silica (silica gel) and crystalline silica polymorphs (quartz, cristobalite and tridymite), as well as calcined kieselguhr, which exhibits both crystalline and amorphous character (IARC 1997).

The structure of crystalline forms of silica can be described as an infinitely repeating lattice. Most natural crystalline silica exists as *α*-quartz, the stable polymorph under ambient conditions, though natural deposits of the metastable polymorphs *α*-tridymite, *α*-cristobalite, coesite, and stishovite are also found (IARC 1997). Conversion between the various metastable silica polymorphs is achievable by heating.

Although most industrial silica is derived from naturally occurring sources, such as silica rich sands and gravels, crystalline forms of silica (mainly quartz) are produced for industrial applications (IARC 1997). Crystalline forms of silica, especially quartz, have a diversity of industrial applications including uses in cat litter, tile mortar, arts, crafts, glass manufacture, ceramic glaze, concrete, and paint (DoEHP QG 2015).

In contrast to crystalline forms of silica, amorphous forms such as silica gel and kieselguhr exhibit only short-range order. Silica gel is produced industrially by acidification of an aqueous sodium silicate solution, and is widely used as a dessicant, and in food production. Kieselguhr is a naturally occurring form of amorphous silica, which consists of the fossilised remains of diatoms, unicellular algae which extract dissolved silica from their environment and use it to form their cell walls. The crystalline silica content of naturally occurring

kieselguhr is 0.1 to 4%, however when it is calcined, up to 65% may be converted to cristobalite (IARC 1997).

The substances in the Silica group include some of the highest volume chemicals used in the Australian coal seam gas industry. Together with water, sand, which is largely composed of silica, makes up 99% of the materials used within hydraulic fracturing fluids (DoEHP QG 2015). Survey information received from the Australian coal seam gas industry indicates that uses of substances in the Silica group are as follows:

- Quartz and cristobalite are used as non-caking aids in drilling fluid formulations and as proppants in hydraulic fracturing or fracturing pre-treatment formulations, with quartz having reported additional uses as a cross-linker and a gel breaker;
- Tridymite is used as a non-caking aid in drilling fluid formulations; and
- Kieselguhr, calcined as a pH buffer, is used as a cross-linker, breaker, surfactant, and clay stabiliser in hydraulic fracturing or pre-treatment formulations.

The uses of silica and silica gel were not specified in the survey information provided. However, silica gel is known to be used to manage the swelling of clays in the vicinity of wells (DoEHP QG 2015).

All forms of silica have low solubility in water, although trace amounts of dissolved silica (silicic acid) are present in almost all terrestrial and aquatic ecosystems across the world (Wetzel 2001). They exhibit no known aquatic ecotoxicity (OECD 2004). Nevertheless, there is potential for members of the Silica group to act as direct, non-toxic physico-chemical stressors by increasing turbidity and decreasing the transfer of light into aquatic ecosystems. However, such impacts should be considered in context, with such turbidity occurring through release and mobilisation of silica and other soil constituents during flood events.

17.3 Chemical name and identification

According to the OECD SIDS Initial Assessment Report for Synthetic Amorphous Silica and Silicates, the substance identified as ‘silica’ in this group which has CAS RN 7631-86-9 is a general identifier for all forms of silica, including synthetic amorphous silica as well as crystalline and natural forms of this oxide (OECD 2004).

CAS Name	**Silica**
CAS RN	7631-86-9
AICS name	Silica
Synonyms	Silicon dioxide
Formula	SiO2

CAS Name	**Silica gel, precipitated, crystalline free**
CAS RN	112926-00-8
AICS name	Silica gel, precipitated, crystalline free
Synonyms	Silicon dioxide Synthetic amorphous silica (SAS) Non-crystalline silica Amorphous precipitated silica Precipitated silica
Formula	SiO2

CAS Name	**Kieselguhr, calcined**
CAS RN	91053-39-3
AICS name	Kieselguhr, calcined
Synonyms	Diatomaceous earth, calcined Diatomite, calcined
Formula	Not applicable

CAS Name	**Quartz (SiO_2)**
CAS RN	14808-60-7
AICS name	Quartz (SiO2)
Synonyms	Silicon dioxide α-Quartz
Formula	SiO2

CAS Name	**Cristobalite (SiO_2)**
CAS RN	14464-46-1
AICS name	Cristobalite (SiO_2)
Synonyms	α-Cristobalite
Formula	SiO_2

CAS Name	**Tridymite (SiO_2)**
CAS RN	15468-32-3
AICS name	Not on AICS
Synonyms	Crystalline silica, Tridymite α-Tridymite
Formula	SiO_2

17.4 Physico-chemical properties

Physico-chemical properties for kieselguhr, calcined (CAS RN: 91053-39-3) were not identified. However, it has been previously noted that calcination of kieselguhr leads to a significant reduction in porosity and specific surface area as compared with the starting kieselguhr, even though some of the biogenic micromorphology of the fossilised diatoms is retained (IARC 1997).

Silica gel, precipitated, crystalline free	
Water solubility	15-68 mg L^{-1} (20°C, at saturation, pH 5.5–6.6 (OECD 2004))
Quartz (SiO_2)	
Melting point	1610°C (Weast 1976)
Density (relative to water)	2.64-2.66 (Weast 1976)
Cristobalite (SiO_2)	
Melting point	1723°C (Weast 1976)
Density (relative to water)	2.32 (Weast 1976)
Crystalline silica, tridymite	
Melting point	1703°C (Weast 1976)
Density (relative to water)	2.26 (Weast 1976)

The substances in the Silica group have low solubility in water, and can only dissolve to maximum concentrations of approximately 60 mg/L (Domenico and Schwartz 1990; Eugster and Jones 1979). Their dissolution or precipitation from solution depends upon the chemistry of the water in which they occur (US EPA 2015), with precipitation and sorption of silica from solution being the main mechanisms limiting dissolved silica concentrations in the environment (Eugster and Jones 1979; OECD 2004).

17.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for substances in the Silica group.

17.6 Environmental fate summary

Silica is the most abundant oxide in the lithosphere, with quartz making up the bulk of sand and silt (CSIRO Division of Soils 1983). The proportion of tridymite, cristobalite, and quartz in

soils reflects the parent rocks from which these minerals originate (CSIRO Division of Soils 1983).

All forms of silica are expected to slowly convert to quartz in soils. This includes silica gel, which has been found to convert to quartz after a month in soil, in the presence of iron, aluminium, and other metals (CSIRO Division of Soils 1983). Amorphous forms of silica occur naturally in soils and originate from decaying plants, although both amorphous silica and crystalline mineral silica play a negligible role in plant nutrition due to their mostly unreactive nature.

Particulate silica and dissolved silica (silicic acids) are present in almost all terrestrial and aquatic ecosystems across the world (OECD 2004). The global average silica concentration in rivers is 13 mg/L with very little variation (Wetzel 2001). Although silica is practicably insoluble due to its highly stable chemical bonds (OECD 2004; Weast 1976), small amounts dissolve to form silicic acid (Wetzel 2001). Silica (in the form of dissolved silicic acid) is an essential nutrient for diatoms, a type of siliceous phytoplankton which dominates phytoplankton populations in many aquatic ecosystems. Diatoms store silica in its amorphous form, using it to form their cell walls. Consumption of silica by siliceous phytoplankton drives aquatic biogeochemical silica cycles (Wetzel 2001).

Large natural fluctuations in silica concentrations occur in lakes with no ecotoxicological effect. These fluctuations may be in response to a range of factors. These include changes to the oxidation-reduction potential of sediments, adsorption of dissolved silica to silica in the solid phase, adsorption of dissolved silica to aluminium and ferric oxyhydroxides, and to a lesser extent diatom uptake (Wetzel 2001). The precipitation of silica from solution and its adsorption to clays are natural mechanisms controlling silica concentrations in rivers (Lindskov and Kimball 1984).

Particulate forms of silica are expected to settle out of the water column into which they are discharged. This settling process is part of the natural process by which the increased turbidity associated with suspended solids (including suspended silica and other mineral and rock particles) in flood waters decreases after a flood event ends.

17.7 Environmental effects summary

Aquatic toxicity studies performed at saturation concentrations of synthetic amorphous silica showed no acute toxicity to fish, *Daphnia*, or algae, though some physical effects were observed with loading rates of greater than or equal to 10 g/L (OECD 2004). Any harmful effects to aquatic ecosystems are therefore not ecotoxicological in nature.

Nevertheless, direct, non-toxic physical stress can occur within aquatic ecosystems if suspensions of amorphous or crystalline silica increase turbidity and disturb normal physico-chemical processes such as photosynthesis (e.g. ANZECC and ARMCANZ 2000; Wetzel 2001). These potential physico-chemical impacts should be considered in context; large volumes of silica are transferred into aquatic ecosystems under normal conditions. For example, the total flux of dissolved silica into the rivers within Western Europe has been estimated to be 4374 kilotonnes per year (Treguet et al. 1995 in: OECD 2004). Potential physico-chemical impacts are considered to be easily mitigated if clean-up occurs immediately after an unintentional release occurs to soil or surface waters.

17.8 Categorisation and other characteristics of concern

17.8.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment (UNECE 2007; US EPA 2007).

17.9 Other characteristics of concern

No chronic aquatic toxicity data were identified for any members of the Silica group. No other characteristics of environmental concern for the substances in this group were identified.

17.10 Screening assessment

17.10.1 Assessment

Substances in the Silica group and their dissolution products are some of the most abundant materials in both aquatic ecosystems and in soils. They have no known aquatic ecotoxicological effects, with dissolved silica concentrations regulated through a range of biogeochemical processes, including precipitation, adsorption, and biological uptake. Moreover, dissolved silica in the form of silicic acid is a critical nutrient for some phytoplankton species.

Amorphous and crystalline forms of silica have low chemical reactivity in the environment, dissolve to a very limited extent, and convert to quartz in most soils. Although particulate silica is considered to have the potential to act as a direct non-toxic physico-chemical stressor if abruptly discharged into aquatic environments, this should be considered in context, with such discharges occurring as a natural process during flood events. Silica particles settle out of the water column as flood waters pass, with a similar outcome considered likely if particulate substances in the Silica group are discharged into the aquatic environment.

Based on the information presented in this report, substances in the Silica group are not considered to be of environmental concern.

17.11 Outcome

A Tier 1 assessment of the environmental risks from the use of substances in the Silica group is not required.

17.12 References

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18 Group assessment – Phyllosilicate rocks and minerals

1302-78-9 Bentonite
14807-96-6 Talc ($Mg_3H_2(SiO_3)_4$)

18.1 Grouping rationale

The phyllosilicate rocks and minerals within the list of 54 materials and chemicals were grouped together for the purposes of this assessment on the basis that they are minerals (or mixtures of minerals) formed through the geological alteration of other rocks and minerals. They are both naturally ubiquitous in the environment and stable on geological timescales.

18.2 Background

Bentonite is a name given to a rock which is a mixture of mostly clay minerals. The main mineral component of bentonite is typically the layered aluminosilicate, montmorillonite, which is one of the smectite group of minerals. Talc is a magnesium silicate mineral. Both minerals are examples of sheet silicates, or phyllosilicates (Deer et al. 1992; WHO 2005).

Many phyllosilicates, including montmorillonite and talc, are secondary minerals that are formed from the geological alteration of pre-existing minerals (CSIRO Division of Soils 1983; Deer et al. 1992; Moore 2001). In the case of the minerals in bentonite, this alteration occurs through weathering of volcanic ash (WHO 2005), while talc is usually formed by hydrothermal processes (Zazenski et al. 1995).

Phyllosilicates are ubiquitous in the environment and occur in differing levels of purity. They are the most important component of vertosols, for example, which are a highly valuable agricultural soil comprised of phyllosilicate minerals including smectite, illite, and kaolinite (McKenzie 2004). Bentonite and talc also occur naturally as mineral deposits within Australia. There are 34 deposits of bentonite and 54 of talc in New South Wales alone. The main New South Wales deposits of bentonite are from the Permian and Carboniferous periods demonstrating the stability of this substance over geological timescales (NSW DPI 2015a and 2015b).

Phyllosilicate rocks and minerals are important global commodities with properties which have multiple applications in a wide range of industries. For example, bentonite has a high cation-exchange capacity and the ability to produce gels with water that have both time and shear dependent viscosity (i.e., they are thixotropic). It also has the ability to absorb a large quantity of water and the substance undergoes considerable swelling in the process. As a result, bentonite is very widely used for sealing dams and the tops of wells, as an ingredient of oil well drilling muds, and in foundry moulding sands (Grim and Güven 1978; WHO 2005). Talc is used as an ingredient in ceramics, cosmetics, as a filler material and lubricant, and as an adsorbent (Deer et al. 1992; NSW DPI 2015b), with 3% of the total talc production used as an ingredient in foods where it can make up one third of the total volume (Zazenski et al. 1995).

Survey information from the Australian coal seam gas industry indicates that bentonite is used as a viscosifier (a substance to increase viscosity) in drilling fluid formulations, while talc is reported to be used as a cross-linker, proppant, or gel breaker in hydraulic fracturing or fracturing pre-treatment formulations.

Phyllosilicate minerals are known to be one of the most significant contributors to inorganic turbidity in aquatic environments (Wetzel 2001). These minerals therefore have some potential to act as a source of direct non-toxic physico-chemical stress in aquatic ecosystems by decreasing the transfer of heat and light.

18.3 Chemical name and identification

CAS Name	**Bentonite**
CAS RN	1302-78-9
AICS name	Bentonite
Synonyms	Bentonite Fuller's earth
Formula	Not applicable
CAS Name	**Talc ($Mg_3H_2(SiO_3)_4$)**
CAS RN	14807-96-6
AICS name	Talc (Mg3H2(SiO3)4)
Synonyms	Talc
Formula	Mg6[(Si8O20](OH)4

18.4 Physico-chemical properties

Bentonite	
Physical form	Plastic solid (WHO 2005)
Melting point	800-900°C (disintegration; WHO 2005)
Density	2.0-2.5 g cm^{-3} (NICNAS 2001)
Cation exchange capacity (montmorillonite)	100 meq/100 g (WHO 2005)
Talc	
Physical form	Foliated or fibrous solid (Deer et al. 1992)
Decomposition point	800-840°C (Ewell et al. 1935)
Density (relative to water)	2.58-2.83 (Deer et al. 1992)

According to the World Health Organisation assessment of bentonite, this material is a highly colloidal and plastic clay (WHO 2005). Montmorillonite, the main clay mineral component of bentonite, occurs as very small crystals which form colloidal suspensions in water. The very small size of montmorillonite crystals results in primary mineral particles with a high surface area that have a much higher cation exchange capacity than some other clay minerals. This has important consequences for the overall properties of bentonite, including its cation exchange capacity and water absorbing/swelling properties (Hunter 1995).

The cation exchange capacity of a mineral (expressed as milliequivalents of monovalent cations per 100 g of dry clay (meq/100 g)) is its ability to exchange cations from the environment with weakly held cations from within the crystal structure of the mineral (Manahan 1990). This capacity is particularly high in clay minerals of the smectite group (WHO 2005). In addition to a relatively high propensity to exchange cations, bentonite is also

a shrink-swell clay and as such has the ability to swell in three dimensions by up to 15 times its original volume upon contact with water (WHO 2005). The combination of its high cation exchange capacity and this shrink-swell property makes bentonite clays highly effective at preventing migration of contaminants from contaminated sites and for sealing dams and reservoirs in general.

Talc also has a high propensity to absorb chemicals, mainly oils and lubricants, and is widely used within industry for this purposes (NSW DPI 2015b; Zazenski et al. 1995).

18.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for unmodified substances in the Phyllosilicate rocks and minerals group.

18.6 Environmental fate summary

Phyllosilicate minerals constitute the major fraction of colloidal minerals found naturally in environmental waters, and they constitute the major cause of all inorganic turbidity in natural waterways (Manahan 1990; Smith 1920; Wetzel 2001). The stability of the clay colloids in water depends on a number of factors, including water chemistry (Hunter 1995; Manahan 1990). However, clay particles can remain suspended in the water column for extended periods where they are responsible for most of the scattering of light from natural water bodies (Wetzel 2001).

In the terrestrial compartment, phyllosilicates are important rock forming minerals and are ubiquitous components of soil. These minerals are stable on geological timescales (CSIRO Division of Soils 1983; McKenzie 2004).

18.7 Environmental effects summary

Phyllosilicate minerals have low toxicity to aquatic species based on the studies reviewed by the World Health Organisation (2005). The principal hazards to the environment from bentonite will arise from excessive turbidity and sedimentation in aquatic ecosystems, physical disturbance to land (e.g. from mining operations or improper disposal), or other similar physically disruptive processes. Talc is similarly expected to have low toxicity to the environmental based on its ubiquity in the environment, its low bioavailability, and its widespread use in consumer products (Zazenski et al. 1995).

18.8 Categorisation and other characteristics of concern

18.8.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals such as phyllosilicate minerals according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment (UNECE 2007; US EPA 2007).

18.8.2 Other characteristics of concern

No other characteristics of environmental concern were identified for substances in the Phyllosilicate rocks and minerals group.

18.9 Screening assessment

18.9.1 Assessment

Phyllosilicate minerals are produced through the geological weathering of rocks over time and they are ubiquitous components of the environment, including most soils and surface waters. They are considered to have low toxicity to aquatic organisms.

There is some potential for bentonite and talc to act as non-toxic, direct physico-chemical stressors by causing an increase in turbidity and thereby decreasing the normal transfer of heat and light into aquatic ecosystems. However, the potential impact should be considered in the context of the natural occurrence of phyllosilicate rocks and minerals, with flood waters carrying high loads of phyllosilicates as part of the natural flooding process. The potential for direct physico-chemical stress in aquatic ecosystems caused by bentonite and talc is considered to be minimal if clean-up occurs immediately after spills or other releases of these solid materials.

18.10 Outcome

A Tier 1 assessment of the environmental risks from the use of substances in the Phyllosilicate rocks and minerals group is not required.

18.11 References

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19 Group assessment – Non-ionic polymers

25038-72-6 2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene
9003-05-8 2-Propenamide, homopolymer

19.1 Grouping rationale

This group is comprised of two synthetic non-ionic polymers. They are both members of the broad category of non-ionic polymers that are generally identified as having similar environmental concerns. These polymers have therefore been assessed as a group.

19.2 Background

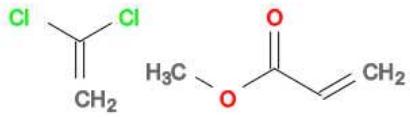
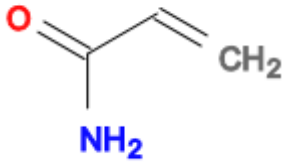
The two substances in this group are both non-ionic synthetic polymers. They are formed by addition polymerisation, which typically affords high molecular weight polymers with stable saturated carbon-chain backbones. These polymers are expected to have a number of domestic and industrial uses, including use as a flocculant in wastewater treatment, thickening agents, suspending agents, and additives in adhesives, food, paints, floor polishes and oil (Beothling and Nabholz 1997; HSDB 2015).

The methacrylate co-polymer in this group (CAS RN: 25038-72-6) has reported uses in hydraulic fracturing or fracturing pre-treatment formulations in Australia as a cross-linker/pH buffer/breaker/surfactant/clay stabiliser. The polyacrylamide homopolymer (CAS RN: 9003-05-8) has reported uses in hydraulic fracturing or fracturing pre-treatment formulations as a scale inhibitor. These polymers were not reported to have uses in drilling fluids. According to international information, polyacrylamides (including the polyacrylamide in this group) are used as friction reducers in so-called ‘slickwater’ fracturing (Stringfellow et al. 2014).

Due to their large size, synthetic addition polymers cannot be absorbed across biological membranes and therefore cannot cause intracellular toxic effects or bioaccumulate. Toxicity typically only occurs through direct surface effects (for example, occlusion of gills), or chelation of essential nutrients. Non-ionic polymers have limited potential to act by either of these modes of action, and are generally considered to be of low ecotoxicological concern to the environment (Beothling and Nabholz 1997).

No information is available regarding the molecular weight and the percentage of low molecular weight (LMW) species in the polymers of this group. However, synthetic addition polymers of this type are generally high to very high molecular weight species. The polymers in this group have therefore been assessed assuming that both polymers have a number average molecular weight (NAMW) greater than 1 000 Da with an insignificant percentage of LMW species.

19.3 Chemical name and identification

CAS Name	2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene	2-Propenamide, homopolymer
CAS RN	25038-72-6	9003-05-8
AICS name	2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene	2-Propenamide, homopolymer
Synonyms	Methyl acrylate-vinylidene chloride copolymer	Polyacrylamide
Monomer formulae		
Formula	(C2H2Cl2)x(C4H6O2)y	(C3H5NO)x
Number Average Molecular Weight (NAMW)	Assumed to be greater than 1000 Da	Assumed to be greater than 1000 Da

19.4 Physico-chemical properties

Property	2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene	2-Propenamide, homopolymer
Physical form	No data	White solid (HSDB 2015)
Melting point	No data	No data
Water solubility	Expected to be low based on the predominantly hydrophobic structure	Highly water soluble (HSDB 2015)
pKa	No dissociable functional groups	No readily dissociable functional groups
Degradation products	Not expected to degrade rapidly under typical environmental conditions	Not expected to degrade rapidly under typical environmental conditions

19.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for these polymers:

Pre-assessment profile	2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene	2-Propenamide, homopolymer
Montreal	No	No
SGG	No	No
Rotterdam	No	No
Stockholm	No	No
REACH (SVHCs)	No	No
EDC (US EPA)	No	No
EDC (Europe)	No	No

19.6 Environmental fate summary

19.6.1 Dissolution, speciation and partitioning

Both polymers in this group have no readily dissociable function groups and they are therefore expected to be non-ionic species in the environment. However, they are expected to have different solubilities in water, which will affect their dissolution and partitioning.

The methylacrylate-vinylidene chloride copolymer is not expected to be highly soluble in water based on its predominantly hydrophobic structure. If discharged to the aquatic environment, this polymer is expected to partition to soil or sediment. It is not expected to be highly mobile if released to the soil compartment (Beothling and Nabholz 1997). However, polyacrylamide is highly soluble in water (HSDB 2015) and is expected to show some partitioning to the water compartment if released to the environment.

19.6.2 Persistence

The polymers in this group are synthetic addition polymers with stable carbon-chain backbones. If released to the environment, the polymers in this group are not expected to undergo rapid degradation, and are considered to be Persistent (P) according to domestic hazard criteria (EPHC 2009).

19.6.3 Bioaccumulation

Polymers with a NAMW greater than 1 000 Da cannot cross biological membranes (Nabholz 1997). Therefore, the polymers in this group are considered to be not bioaccumulative (Not B) according to domestic hazard criteria (EPHC 2009).

19.6.4 Transport

The polymers in this group are not expected to undergo long-range transport in the environment.

19.7 Environmental effects summary

No relevant toxicity data for these two polymers were identified.

Non-ionic polymers with low water solubility, such as the methyl acrylate-vinylidene chloride copolymer, generally have low toxicity to aquatic life (Beothling and Nabholz 1997). Insoluble non-ionic polymers have low bioavailability and their adverse effects result from physical

effects such as occlusion of respiratory organs (e.g. the gills of fish). These adverse effects occur only at very high loading levels in water (Beothling and Nabholz 1997).

Water soluble or dispersible non-ionic polymers, such as polyacrylamide, are also typically of low concern for ecotoxicity. Non-ionic polymers with NAMW greater than 1 000 cannot be absorbed across biological membranes in aquatic organisms, and therefore toxicity only occurs through indirect effects such as chelation of essential nutrients (Beothling and Nabholz 1997). However, the structure of polyacrylamide suggests that it will have low potential to act by this mode of action. This is further supported by median effective concentration (EC50) and median lethal concentration (LC50) values available for other water soluble or dispersible non-ionic polymers, which are greater than 100 mg/L (Beothling and Nabholz 1997).

Water soluble or dispersible polymers with NAMW less than 1 000 Da, or significant levels of LMW substances and trapped monomers, are of potential concern because of their increased bioavailability. However, this assessment was conducted assuming that the polymers in this group have NAMW greater than 1 000 Da and the percentage of LMW species is low.

Both polymers in this group are categorised as not toxic (Not T) according to domestic environmental hazard criteria (EPHC 2009).

19.8 Categorisation and other characteristics of concern

19.8.1 PBT categorisation

The polymers in this group are not PBT substances according to domestic environmental hazard criteria.

19.8.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for these polymers.

19.9 Screening assessment

19.9.1 Assessment

The two polymers in this group are stable non-ionic polymers which are used in a range of domestic and industrial applications. High molecular weight synthetic non-ionic polymers of this type are generally considered to be of low concern to the environment (Beothling and Nabholz 1997). They are not bioaccumulative and have low direct toxicity to aquatic organisms. They are expected to be persistent in the environment, although they generally have low mobility and very low bioavailability.

Adverse effects from the parent non-ionic polymers in this group are only likely to occur at very high loading levels in the aquatic environment where, for example, the polymers may physically block respiratory organs. Such loading levels in the aquatic environment are only expected to have potential to occur in the event of very large accidental spills. However, any such spills are expected to be cleaned up before these polymers can be released to surface waters.

19.10 Outcome

A Tier 1 assessment of the environmental risks from the use of the polymers in the non-ionic polymers group is not required.

19.11 References

Boethling, RS, and Nabholz, JV 1997, 'Environmental assessment of polymers under the US Toxic Substances Control Act*',* in Hamilton J and Sutcliffe R (eds), *Ecological assessment of polymers: strategies for product stewardship and regulatory programs*, Van Nostrand Reinhold, New York, USA, pp 187-234.

EPHC 2009, Environmental risk assessment guidance manual for industrial chemicals, Environment Protection and Heritage Council, Canberra, retrieved from <http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals>

HSDB 2015, 'Polyacrylamide', TOXNET Toxicology data network, viewed 15 August 2015 <http://toxnet.nlm.nih.gov/cgi-bin/sis/search2/f?./temp/~UAQMpv:1>.

Stringfellow, WT, Domen, JK, Camarillo, MK, Sandelin, WL and Borglin, S 2014, 'Physical, chemical, and biological characteristics of compounds used in hydraulic fracturing', *Journal of Hazardous Materials*, vol. 275, pp. 37-54.

20 Group assessment – Anionic polymers

9003-06-9 2-Propenoic acid, polymer with 2-propenamide
CBI Polymer I
CBI Polyacrylamide/polyacrylate copolymer

Confidentiality from public disclosure was claimed for the name and Chemical Abstracts Service Registry Number (CAS RN) of two polymers. Information about the polymers subject to commercial-in-confidence claims was provided to the assessment team and a detailed screening assessment of the polymers was conducted. The polymers, for which confidentiality was claimed, are referred to as 'polymer I' and 'polyacrylamide/polyacrylate copolymer' hereafter, respectively.

20.1 Grouping rationale

This group contains a synthetic copolymer of acrylic acid and acrylamide and two similar polymers. All will dissociate into similar anionic copolymers if discharged to the aquatic environment. They are therefore expected to have similar environmental concerns and have consequently been assessed as a group.

20.2 Background

The three polymers in this group are anionic (or potentially anionic) synthetic copolymers. They are formed by addition polymerisation, which typically affords high molecular weight polymers with stable saturated carbon-chain backbones. All three polymers are expected to dissociate in water to release similar high molecular weight polyanions and simple counterions.

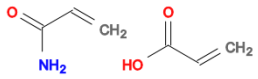
The polymers in this group are reported to be used industrially as thickening agents, viscosity adjustors, filling agents, cleaning/washing agents, polishing agents, foam-reducing agents, surfactants and detergents, paints, lacquers and varnishes, adhesives, binding agents, in the extraction of crude petroleum and natural gas, and as a raw material for production of paper (US EPA 2015).

All three polymers are reported to have uses in Australia in drilling fluid formulations as scale inhibitors. These polymers were not reported to have domestic uses in fracturing or fracturing pre-treatment formulations. According to international information, polyacrylamides (including anionic polyacrylamides) are used as friction reducers in so-called 'slickwater' fracturing (Stringfellow et al. 2014).

Due to their large size and negative charge, anionic polymers cannot cross biological membranes. The polymers therefore cannot cause intracellular toxic effects or bioaccumulate (Boethling and Nabholz 1997). On this basis, anionic polymers generally have low toxicity to fish and aquatic invertebrates. However, anionic polymers may have moderate toxicity to algae because they have the potential to over-chelate Ca^{2+} and Mg^{2+} cations which are nutrients needed for growth (Boethling and Nabholz 1997). This mode of toxic action is directly related to the carbon distance between acid functional groups on the polymer backbone. The highest toxicity occurs when the acid is on alternating carbons of the polymer backbone.

No information is available regarding the molecular weight and the percentage of low molecular weight (LMW) species in the polymers of this group. However, synthetic addition polymers of this type are generally high to very high molecular weight species. The polymers in this group have been assessed assuming that the polymers have a number average molecular weight (NAMW) greater than 1 000 Da with an insignificant percentage of LMW species.

20.3 Chemical name and identification

CAS Name	**2-Propenoic acid, polymer with 2-propenamide**	**CBI**	**CBI**
CAS RN	9003-06-9	CBI	CBI
AICS name	2-Propenoic acid, polymer with 2-propenamide	Not presented	Not presented
Synonyms	Acrylic acid-acrylamide copolymer	Not presented	Not presented
Monomer structural formulae		Not presented	Not presented
Formula	$(C_3H_5NO)_x(C_3H_4O_2)_y$	Not presented	Not presented
Number Average Molecular Weight (NAMW)	Assumed to be greater than 1 000 Da	Assumed to be greater than 1 000 Da	Assumed to be greater than 1 000 Da

20.4 Physico-chemical properties

Property	**2-Propenoic acid, polymer with 2-propenamide**	**Polymer I**	**Polyacrylamide/polyacrylate copolymer**
Physical form	No data	No data	No data
Melting point	No data	No data	No data
Water solubility	Expected to be water soluble based on predominately hydrophilic structure	Expected to be water soluble based on predominately hydrophilic structure	Expected to be water soluble based on predominately hydrophilic structure
pK_a	Contains dissociable functional groups and has potential to be negatively charged	Contains dissociable functional groups and has potential to be negatively charged	Contains dissociable functional groups and has potential to be negatively charged

Property	2-Propenoic acid, polymer with 2-propenamide	Polymer I	Polyacrylamide/polyacrylate copolymer
Degradation products	Not expected to degrade rapidly under typical environmental conditions	Not expected to degrade rapidly under typical environmental conditions	Not expected to degrade rapidly under typical environmental conditions

20.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for these polymers:

Pre-assessment profile	2-Propenoic acid, polymer with 2-propenamide	Polymer I	Polyacrylamide/polyacrylate copolymer
Montreal	No	No	No
SGG	No	No	No
Rotterdam	No	No	No
Stockholm	No	No	No
REACH (SVHCs)	No	No	No
EDC (US EPA)	No	No	No
EDC (Europe)	No	No	No

20.6 Environmental fate summary

20.6.1 Dissolution, speciation and partitioning

The polymers in this group are expected to be water soluble based on their predominately hydrophilic structure. In water, they are expected to dissociate to release similar high molecular weight polyanions based on the typical acidity of the functional group moieties present in each polymer.

The partitioning behaviour of water soluble polyanions is complex and depends on both the exposure conditions and the structure and size of the polymer. For example, up to 90% of very high molecular weight polyanions (NAMW > 50 000 Da) are expected to be removed in waste water treatment plants through partitioning to sewage sludge. The removal efficiency for lower molecular weight water-soluble polyanions (NAMW < 5 000 Da) is only up to 50% (Boethling and Nabholz 1997). The polyanions in this group are expected to partition onto natural colloids in surface waters and in soil.

20.6.2 Persistence

The polymers in this group are synthetic addition polymers with stable carbon-chain backbones. If released to the environment, the polymers in this group are not expected to

undergo rapid degradation, and are considered to be Persistent (P) according to domestic hazard criteria (EPHC 2009).

20.6.3 Bioaccumulation

Polymers with a NAMW greater than 1 000 Da cannot cross biological membranes (Boethling and Nabholz 1997). Therefore, the polymers in this group are considered to be not bioaccumulative (Not B) according to domestic hazard criteria (EPHC 2009).

20.6.4 Transport

The polymers in this group are not expected to undergo long-range transport in the environment.

20.7 Environmental effects summary

No specific ecotoxicity data for the three polymers in this group were identified. However, they are not expected to have significant ecotoxicological effects in the environment.

High molecular weight anionic polymers (including water-soluble polyanions) generally have low toxicity to fish and aquatic invertebrates. These polymers cannot be absorbed across biological membranes in aquatic organisms, and therefore toxicity only occurs through indirect effects such as chelation of essential nutrients. This is supported by median lethal concentration (LC50) values available for anionic polymers which are typically greater than 100 mg/L (Boethling and Nabholz 1997).

Water soluble or dispersible anionic polymers may be moderately toxic to algae because they have the potential to over-chelate Ca^{2+} and Mg^{2+} cations which are essential nutrients needed for growth (Boethling and Nabholz 1997). Toxicity by this mechanism is directly related to the carbon distance between acid functional groups. The highest toxicity occurs when the acid is on alternating carbons of the polymer backbone and homopolymers of acrylic acid generally have the highest indirect toxicity to algae for this reason (Boethling and Nabholz 1997).

The polymers in this group may have some potential to chelate Ca^{2+} and Mg^{2+} cations if they have a significant number of repeating acid units in the polymer structure. However, the toxicity to algae is likely to be reduced under most circumstances due to the presence of background concentrations of calcium ions in most applications, which will bind to the chelating residues in the polymers before they are released to the environment. Even under optimal conditions for toxicity of homopolymers of acrylic acid, the measured median effect concentration (EC50) values for these indirect toxicity effects to algae are greater than 3 mg/L (Boethling and Nabholz 1997).

Water-soluble or dispersible polymers with NAMW less than 1 000 Da, or significant levels of LMW substances and trapped monomers, are of concern because of their bioavailability. However, this assessment is conducted assuming that the polymers have NAMW greater than 1 000 Da and the percentage of LMW species is low.

The polymers in this group are categorised as not toxic (Not T) to aquatic life according to domestic toxicity criterion (EPHC 2009).

20.8 Categorisation and other characteristics of concern

20.8.1 PBT categorisation

The polymers in this group are not PBT substances according to domestic environmental hazard criteria.

20.8.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for the polymers in this group.

20.9 Screening assessment

20.9.1 Assessment

The three polymers in this group are stable synthetic copolymers which are widely used in a range of domestic and industrial applications. High molecular weight polyanions such as those in this group are generally considered to have low toxicity to aquatic organisms. They are not bioaccumulative and have low toxicity to fish and aquatic invertebrates. Although these polymers may have some potential to be indirectly toxic to algae as a result of overchelation of essential cations, this toxicity is expected to be reduced due to complexation of calcium ions by the polymers before they enter the aquatic environment.

20.10 Outcome

A Tier 1 assessment of the environmental risks from the use of the polymers in the Anionic polymers group is not required.

20.11 References

Boethling RS, and Nabholz JV 1997, 'Environmental assessment of polymers under the US Toxic Substances Control Act*',* in Hamilton J and Sutcliffe R (eds), *Ecological assessment of polymers: strategies for product stewardship and regulatory programs*, Van Nostrand Reinhold, New York, USA, pp 187-234.

EPHC 2009, Environmental risk assessment guidance manual for industrial chemicals, Environment Protection and Heritage Council, Canberra, retrieved from <http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals>.

Stringfellow, WT, Domen, JK, Camarillo, MK, Sandelin, WL and Borglin, S 2014, 'Physical, chemical, and biological characteristics of compounds used in hydraulic fracturing', *Journal of Hazardous Materials*, vol. 275, pp. 37–54.

US EPA 2015, *Aggregated computational toxicology resource*, retrieved from <http://actor.epa.gov/actor/faces/ACToRHome.jsp;jsessionid=D00F154E529B41EFF0264E4F24FA062E>.

21 Group assessment – Cationic polymers

26062-79-3 2-Propen-1-aminium, *N*,*N*-dimethyl-*N*-2-propenyl-, chloride, homopolymer

CBI Polyamine

Confidentiality from public disclosure was claimed for the name and Chemical Abstracts Service Registry Number (CAS RN) of one polymer. Information about the polymer subject to commercial-in-confidence claims was provided to the assessment team and a detailed screening assessment of the polymer was conducted. The polymer, for which confidentiality was claimed, is referred to as the 'polyamine' hereafter.

21.1 Grouping rationale

The two polymers in this group are either cationic or expected to be cationic under environmental conditions. The toxicity of cationic polymers to aquatic organisms generally involves a similar mode of action, and they have generally similar environmental fate characteristics. These two polymers have therefore been assessed as a group.

21.2 Background

The two polymers in this group are synthetic homopolymers that are (or are expected to be) cationic under environmental conditions. They have a number of domestic and industrial uses, including as cleaning/washing agents, coagulating agents, emulsion-inhibiting agents, metal surface coating agents, paint additives, flocculating chemicals, paper manufacture chemicals, and fixing agents. They are used in paints, lacquers and varnishes, cutting fluids, and cosmetics (US EPA 2015).

The diallyldimethylammonium chloride homopolymer (CAS RN: 26062-79-3) has reported uses in hydraulic fracturing in Australia for clay control. The remaining polymer in this group is reported to be used as a placement aid/flow and conductivity enhancer in hydraulic fracturing. These polymers were not reported to have domestic uses in drilling fluid formulations.

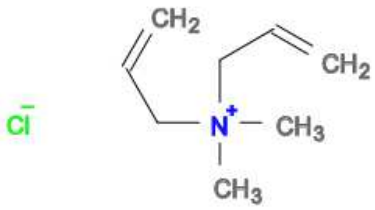
High molecular weight polymers cannot be absorbed across biological membranes due to their large size. Hence, high molecular weight polymers cannot cause intracellular toxic effects or bioaccumulate. However, the polymers in this group are expected to be present as polycations in the environment. Cationic polymers adsorb to negatively charged biological membranes and can cause toxic effects to biota. The toxicity of cationic polymers is most strongly influenced by charge density and the type of polymer backbone. The presence of dissolved organic carbon and suspended solids is known to significantly mitigate the toxicity of cationic polymers under typical environmental exposure conditions (Boethling and Nabholz 1997).

The manufacture of polymers can result in the production of macromolecules with a range of molecular weights. The proportion of low molecular weight (LMW) species is important to consider, as substances with a number average molecular weight (NAMW) less than 1 000 Da can have different properties. Limited information was available regarding the molecular weight and percentage of LMW species for the polymers in this group. The

polymers in this group have been assessed assuming that they have a NAMW greater than 1 000 Da with an insignificant percentage of LMW species.

The diallyldimethylammonium chloride homopolymer will dissociate into polyammonium cations and chloride anions in the aquatic environment. Chloride ions are an essential constituent of electrolytes in all biological fluids responsible for maintaining acid/base balance, transmitting nerve impulses and regulating fluid in and out of cells (NCBI 2015). The concentration of chloride ions is naturally regulated within organisms. The information presented in this assessment has therefore focused on the environmental fate and effects of the synthetic polyamine and polyammonium constituents of the substances in this group.

21.3 Chemical name and identification

CAS Name	**2-Propen-1-aminium, *N*,*N*-dimethyl-*N*-2-propen-1-yl-, chloride (1:1), homopolymer**	**CBI**
CAS RN	26062-79-3	CBI
AICS name	2-Propen-1-aminium, *N*,*N*-dimethyl-*N*-2-propenyl-, chloride, homopolymer	Not presented
Synonyms	Diallyldimethylammonium chloride homopolymer DADMAC homopolymer	Not presented
Monomer formula		Not presented
Formula	$(C_8H_{16}N.Cl)x$	Not presented
Number Average Molecular Weight (NAMW)	Assumed to be greater than 1 000 Da	Assumed to be greater than 1 000 Da

21.4 Physico-chemical properties

Property	**2-Propen-1-aminium, *N*,*N*-dimethyl-*N*-2-propenyl-, chloride, homopolymer**	**Polyamine**
Physical form	Solid (US EPA 2015)	Variable, depending on structure (US EPA 2015)
Melting point	No data	No data
Water solubility	Expected to be water soluble (or water dispersible) based on the predominately hydrophilic structure of the polymer backbone	Expected to be water soluble based on the predominately hydrophilic structure of the polymer backbone

Property	2-Propen-1-aminium, *N,N*-dimethyl-*N*-2-propenyl-, chloride, homopolymer	Polyamine
pK_a	Contains quaternary ammonium units which impart a permanent positive charge to the polymer chain	Contains basic amine nitrogens in the polymer backbone which have the potential to become protonated (i.e. cationic) under environmental conditions
Degradation products	Not expected to degrade rapidly under environmental conditions	Not expected to degrade rapidly under environmental conditions

21.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for these polymers:

Pre-assessment profile	2-Propen-1-aminium, *N,N*-dimethyl-*N*-2-propenyl-, chloride, homopolymer	Polyamine
Montreal	No	No
SGG	No	No
Rotterdam	No	No
Stockholm	No	No
REACH (SVHCs)	No	No
EDC (US EPA)	No	No
EDC (Europe)	No	No

21.6 Environmental fate summary

21.6.1 Dissolution, speciation and partitioning

The polymers in this group are expected to be soluble in water (or water dispersible) based on their predominately hydrophilic structure. The diallyldimethylammonium chloride homopolymer is a permanent polycation based on the presence of quaternary ammonium units in the polymer structure. The other polymer in this group contains basic amine units that are therefore expected to be protonated in water to also form a polycation. Cationic polymers strongly sorb to negatively charged surfaces. As a consequence, both polymers will bind to particulate organic matter and mineral particles and hence predominately partition to the soil and sediment compartments. In these compartments, cationic polymers are expected to be immobile based on their high molecular weight and positive charges (Boethling and Nabholz 1997).

21.6.2 Persistence

The polymers in this group are synthetic polymers, which are typically persistent in the environment (Boethling and Nabholz 1997). Structural information available for the polymers in this group indicates low potential for degradation. If released to the environment, the

polymers in this group are not expected to undergo rapid degradation, and are considered to be persistent (P) according to domestic hazard criteria.

21.6.3 Bioaccumulation

Polymers with a NAMW greater than 1 000 Da cannot cross biological membranes (Boethling and Nabholz 1997). Therefore, the polymers in this group are considered to be not bioaccumulative (Not B) according to domestic hazard criteria.

21.6.4 Transport

The polymers in this group are not expected to undergo long-range transport in the environment.

21.7 Environmental effects summary

21.7.1 Critical environmental effects

Polymers that are cationic in the environment can cause toxic effects in aquatic organisms due to their ability to bind to negatively charged biological membranes. The toxicity of these polymers is related to their number of charges per unit of molecular weight, commonly referred to as charge density, as well as the structure of the polymer backbone type. Cationic polymers with carbon-based backbones and high charge densities appear to be most toxic to aquatic organisms, with median effective (or lethal) concentration (E(L)C50) values as low as 0.016 mg/L determined in tests with algae (Boethling and Nabholz 1997).

However, under environmental conditions, the toxicity of these polymers is mitigated by the presence of dissolved organic carbon (DOC) and suspended solids. Cationic polymers react with DOC in environmental waters to form insoluble complexes, which settle out of water and therefore are not bioavailable to cause toxic effects. It has previously been established that a reduction in likely toxicity by a factor of 110 is appropriate to apply to laboratory test results for cationic polymers with a high charge density to account for the mitigating effects of DOC on toxicity in natural environmental waters (Boethling and Nabholz 1997).

21.7.1.1 Acute toxicity endpoints for aquatic organisms

No measured ecotoxicological data are available for the polymers in this group.

In the absence of measured data for these polymers, their aquatic toxicity has been estimated based on the charge density of the polymer according to Nabholz and Boethling (1997). The charge density for these polymers, measured as percent amine-nitrogen, was determined to be 8.7% and 32.5% for diallyldimethylammonium chloride homopolymer and the remaining polymer (assuming protonation of all available basic nitrogens), respectively. Using these values, and noting that for both polymers the percent amine-nitrogen exceeds 3.5, the acute toxicity of these polymers was estimated using the standard structure-activity relationship as outlined by Nabholz and Boethling (1997):

Taxon	Endpoint	Method
Fish	96 h LC50 = 0.28 mg/L	Calculated (Boethling and Nabholz 1997)
Invertebrates	48 h EC50 = 0.10 mg/L	Calculated (Boethling and Nabholz 1997)
Algae	96 h EC50 = 0.04 mg/L	Calculated (Boethling and Nabholz 1997)

Based on these values, the polymers in this group are considered toxic (T) according to domestic hazard criteria. However, the toxicity of these polymers in the environment is expected to be mitigated by the presence of DOC. Based on the high charge density of the polymers in this group, a standard mitigation factor of 110 was applied to the above calculated toxicity values (Boethling and Nabholz 1997):

Taxon	Mitigated Endpoint	Method
Fish	96 h LC50 = 30.8 mg/L	Calculated (Boethling and Nabholz 1997)
Invertebrates	48 h EC50 = 11.0 mg/L	Calculated (Boethling and Nabholz 1997)
Algae	96 h EC50 = 4.4 mg/L	Calculated (Boethling and Nabholz 1997)

These mitigated toxicity values indicate that the polymers in this group will have only slight to moderate toxicity to aquatic organisms under typical environmental conditions where dissolved organic carbon and suspended solids are ubiquitous components of natural water bodies.

21.8 Categorisation and other characteristics of concern

21.8.1 PBT categorisation

The polymers in this group are not PBT substances according to domestic environmental hazard criteria.

21.8.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for these polymers.

21.9 Screening assessment

21.9.1 Assessment

The two polymers in this group are used in a wide range of domestic and industrial applications. In the environment, they are expected to be present as polycations with high charge densities. These cationic polymers are expected to be persistent and not bioaccumulative. If released to surface soil, they are expected to be highly immobile and have limited bioavailability. If released to surface waters, these polymers are again expected to predominantly partition out of water to sediment where they will not be bioavailable.

Cationic polymers can be highly toxic to aquatic organisms due to their potential to bind to negatively charged biological membranes. Under typical environmental conditions, the toxicity of low concentrations of these polymers is expected to be mitigated by their partitioning behaviour and the presence of naturally occurring DOC and suspended solids, which significantly reduces the bioavailability of the polymers to aquatic biota. Release of large volumes of these polymers directly to surface water may overwhelm these mechanisms and lead to toxic effects. However, spills of such large volumes are expected to be cleaned up before considerable release to surface waters can occur.

21.10 Outcome

A Tier 1 assessment of the environmental risks from the use of the substances in the Cationic polymers group is not required.

21.11 References

Boethling, RS, and Nabholz, JV 1997, 'Environmental assessment of polymers under the US Toxic Substances Control Act', in Hamilton J and Sutcliffe R (eds), *Ecological assessment of polymers: strategies for product stewardship and regulatory programs*, Van Nostrand Reinhold, New York, USA, pp 187-234.

NCBI 2015, *Chloride, PubChem ID 312*, National Center for Biotechnology Information, USA, viewed 2 September 2015 <http://pubchem.ncbi.nlm.nih.gov/compound/chloride#section=Top>.

US EPA 2015, *Aggregated computational toxicology resource,* retrieved from <http://actor.epa.gov/actor/faces/ACToRHome.jsp;jsessionid=D00F154E529B41EFF0264E4F24FA062E>.

22 Group assessment – Modified celluloses

9004-62-0 Cellulose, 2-hydroxyethyl ether
Not supplied Polyanionic cellulose (PAC)
CBI Polysaccharide

22.1 Grouping rationale

The screening assessment of these three polymers has been conducted as a group because they are all chemically modified celluloses. They all have similar properties and are expected to share a very similar fate if released into the environment.

22.2 Background

Cellulose is a polysaccharide biopolymer that consists of several hundred to thousands of β(1→4) linked D-glucose units in a linear chain (Chen 2014). It is produced by green plants and algae and is the most abundant renewable organic substance in nature (de Oude 1992). Cellulose is completely insoluble in water, but it can be chemically modified to increase its solubility. All of the substances in this group are chemically modified celluloses.

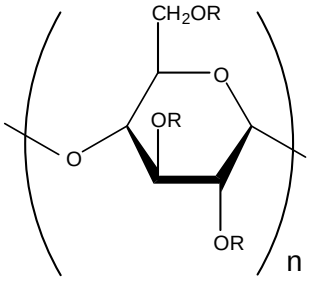
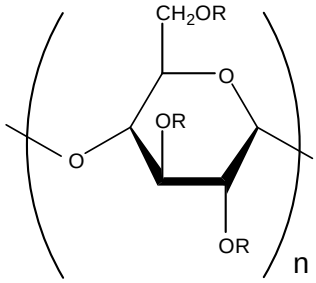
According to industry information, polyanionic cellulose (PAC) is similar in structure, properties and usage to carboxymethyl cellulose (US EPA 2013a). The latter polymer has numerous uses in food (WHO and FAO 2015) and in laundry formulations (de Oude 1992). The other polymers in this group have a variety of industrial uses such as surface-active agents, viscosity adjustors, cleaning/washing agents, fillers, adhesives and binding agents, construction materials (Nordic Council of Ministers 2015), and they also have therapeutic uses (US NLM 2013).

The polymers in this group are reported to have uses in drilling fluid formulations for fluid loss control and as a gelling agent during fracturing or fracturing pretreatment. Fluid loss control chemicals are used to stop drilling fluids escaping into the formation by way of crevices or porous media (Bucksch 2013). Gelling agents are used to increase the viscosity of fracturing fluids, allowing for better proppant suspension and transport into developed fractures. Gelling compounds are dissolved into a non-aqueous solvent for addition to the fracturing fluid up to a final concentration in the range 10 to 1000 mg/L (Stringfellow et al. 2014).

Release of significant volumes of these polymers directly to aquatic ecosystems may cause temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations as the polymers are degraded by microorganisms. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate concentrations of these polymers in aquatic ecosystems.

22.3 Chemical name and identification

Based on available industry information, the substance identified as polyanionic cellulose (PAC) is similar in structure, properties and usage in drilling fluids to the industrially important semi-synthetic cellulose polymer, carboxymethyl cellulose (US EPA 2013a). Carboxymethyl cellulose (CMC) has therefore been used as an analogue for PAC in this assessment.

CAS Name	**Cellulose, 2-hydroxyethyl ether**	**Cellulose, carboxymethyl ether** **(Analogue)**
CAS RN	9004-62-0	9000-11-7
AICS name	Cellulose, 2-hydroxyethyl ether	Cellulose, carboxymethyl ether
Synonyms	Hydroxyethylcellulose HEC	Carboxymethyl cellulose Cellulose gum CMC
Structure	 R = H or CH2CH2OH	 R = H or CH2COOH
Number Average Molecular Weight (NAMW)	Assumed to be greater than 1 000	Assumed to be greater than 1 000

The main parameters used to characterise modified celluloses are the degree of substitution (DS) (average number of hydroxyl groups replaced by substituents) and the degree of polymerisation (DP) (the number of monomeric units in the polymer) (de Oude 1992; Varshney and Naithani 2011). The maximum DS is 3 for cellulose.

No information is available regarding the molecular weight and the percentage of low molecular weight (LMW) oligomers and other species present as impurities in these polymers. For the purposes of this assessment, the polymers in this group have been assumed to have a number average molecular weight (NAMW) greater than 1 000 Da with an insignificant percentage of LMW species. Modified celluloses are typically very high molecular weight species, for example, CMC production requires pure cellulose with a DP up to 6 000 (de Oude 1992).

22.4 Physico-chemical properties

Property	**Cellulose, 2-hydroxyethyl ether (HEC)**	**Cellulose, carboxymethyl ether (CMC)**
Physical form	White, free flowing powder (US NLM 2013)	No data
Melting point	140°C (US EPA 2013b)	No data
Water solubility	Water soluble (Reese et al. 1950)	Water soluble (de Oude 1992)
pKa	No readily dissociable functional groups	Expected to be present in the environment as a polyanion as a result of the ionisation of the carboxymethyl substituents

Hydroxyethyl cellulose is water soluble (Reese et al. 1950). The available information indicates that commercially available CMC typically has a DS > 0.5 and will therefore also be water soluble (de Oude 1992; Varshney and Naithani 2011).

22.5 Domestic and international regulatory information

A review of international and national environmental regulatory information was undertaken. No specific environmental regulatory controls or concerns were identified within Australia and internationally for the polymers in this group:

Pre-assessment profile	
Montreal	No
SGG	No
Rotterdam	No
Stockholm	No
REACH (SVHCs)	No
EDC (US EPA)	No
EDC (Europe)	No

22.6 Environmental fate summary

22.6.1 Dissolution, speciation and partitioning

All of the polymers in this group are expected to be water soluble. If discharged into natural waters, CMC is expected to be present as a polyanion as a result of the ionisation of the carboxymethyl substituents. Hydroxyethyl cellulose is not expected to dissociate in water as it has no readily dissociable functional groups.

The polymers in this group may show comparatively complex partitioning behaviour in aquatic systems based on the well-established interactions between colloids and CMC, which is a key part of the function of this polymer in laundry detergents (de Oude 1992).

22.6.2 Persistence

The polymers in this group have Uncertain Persistence (Uncertain P) according to domestic hazard criteria (EPHC 2009).

In the environment, the biodegradation of CMC is initiated by naturally occurring extracellular enzymes followed by the mineralisation of monomeric and oligomeric saccharides by microorganisms (de Oude 1992). Biological oxygen demand (BOD) tests (used to measure biodegradation by aerobic mixed cultures) are usually limited to four weeks. However, after an adaptation of 16 weeks, highly substituted CMC was biodegraded with no stable intermediates produced (de Oude 1992). Therefore, if the polymers in this group are released to surface waters or soil they are expected to eventually biodegrade into water and oxides of carbon.

Although the polymers in this group are expected to be ultimately degradable in the environment, the rate of biodegradation is variable and sensitive to the degree of chemical modification. In BOD tests, CMC (DS 0.4-0.5) was found to be partially oxidised while CMC (DS 1.2-1.4) was found to be recalcitrant (de Oude 1992). Commercially available CMC

typically has a DS >0.5 and hence its potential to rapidly biodegrade in the environment is uncertain.

22.6.3 Bioaccumulation

The polymers in this group are Not Bioaccumulative (Not B) according to domestic hazard criteria (EPHC 2009).

No bioaccumulation data were available for the polymers in this group. Assuming their NAMW is greater than 1 000, the polymers in this group will be unable to cross cell membranes and are therefore not expected to be bioaccumulative (Boethling and Nabholz 1997).

22.6.4 Transport

The polymers in this group are non-volatile and they will eventually biodegrade in the environment. Therefore, the polymers in this group are not expected to undergo long-range transport.

22.7 Environmental effects summary

22.7.1 Critical environmental effects

22.7.1.1 Acute toxicity endpoints for aquatic organisms

The polymers in this group are Not Toxic (Not T) according to domestic hazard criteria (EPHC 2009).

Hydroxyethyl cellulose is a water soluble non-ionic polymer. Polymers of this type with a NAMW greater than 1 000 generally have low acute toxicity to aquatic life and are therefore of low concern for ecotoxicity (Boethling and Nabholz 1997).

The following measured median effective concentration (EC50) and median lethal concentration (LC50) values for model organisms were identified for the sodium salt of CMC, which has been used as analogue for CMC. The endpoints were obtained from databases in the OECD QSAR Toolbox (LMC 2013):

Taxon	Endpoint	Method
Fish	96 h LC50 > 20 000 mg/L	Experimental Oncorhynchus mykiss and Carassius carassius
Invertebrates	48 h EC50 = 87.3 mg/L	Experimental Ceriodaphnia affinis
Algae	Not available	-

No ecotoxicological data were identified for the effects of CMC or sodium CMC on algae. Both of these polymers will be polyanions under typical conditions in aquatic ecosystems. Some polyanions are known to be moderately toxic to algae. The mode of toxic action is over-chelation of nutrient elements needed by algae for growth. The highest toxicity is when there is an acid group on alternating carbons of the polymer backbone. This will not apply to the polymers in this group and they are therefore not considered to be an over-chelation hazard to algae (Boethling and Nabholz 1997).

22.7.1.2 Chronic toxicity endpoints for aquatic organisms

No chronic ecotoxicity data for the polymers in this group were identified.

22.8 Categorisation and other characteristics of concern

22.8.1 PBT categorisation

The polymers in this group are not PBT substances according to domestic environmental hazard criteria.

22.8.2 Other characteristics of concern

No other characteristics of concern for the environment were identified for the polymers in this group.

22.9 Screening assessment

22.9.1 Assessment

The polymers in this group are chemically modified celluloses. Hydroxyethyl cellulose is expected to remain as a non-ionic polymer in surface waters under typical exposure conditions, while CMC is expected to ionise into an anionic polymer. If released to the environment the polymers are not expected to be toxic or bioaccumulative to aquatic or terrestrial organisms. Eventually the polymers will be biodegraded by naturally occurring extracellular enzymes into simple sugars, which will in turn be rapidly consumed by microorganisms in the environment.

Release of significant volumes of these polymers directly to aquatic ecosystems may cause temporary changes in water quality for local organisms, such as reduced dissolved oxygen concentrations as the polymers are degraded by microorganisms. However, normal biogeochemical regulation mechanisms are expected to be able to limit the effects of moderate concentrations of these polymers in aquatic ecosystems. Spills of larger volumes of these polymers are expected to be cleaned up before they can be released to surface waters.

22.10 Outcome

A Tier 1 assessment of the environmental risks from the use of the polymers in the Modified celluloses group is not required.

22.11 References

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23 Group assessment – Enzymes

9012-54-8 Cellulase
9025-56-3 Hemicellulase
CBI Enzyme

Confidentiality from public disclosure was claimed for the name and Chemical Abstracts Service Registry Number (CAS RN) of one enzyme. Information about the enzyme subject to commercial-in-confidence claims was provided to the assessment team and a detailed screening assessment of the enzyme was conducted. The enzyme, for which confidentiality was claimed, is referred to as 'enzyme' hereafter.

23.1 Grouping rationale

Cellulase, hemicellulase, and the enzyme were assessed as a group based on their function, biochemical properties, natural occurrence and use in the coal seam gas industry. The purpose of this assessment is to establish whether they could cause any potential harm when released into the environment. The results of this assessment are presented below.

23.2 Background

The natural function of the substances in this group is to degrade cellulose and hemi-cellulose. Cellulose and hemi-cellulose are important structural components of green plants where they can be found in the cell walls (Klemm et al. 2005; Sjöström 1993). They are biopolymers consisting of several hundred to several thousand sugar monomers such as glucose and mannose, and can make up to 60% of wood dry weight (Sjöström 1993). Cellulose is the most abundant organic polymer on Earth with an estimated annual global production of 10^{11} to 10^{12} tons by photosynthesis (Krässig 1993).

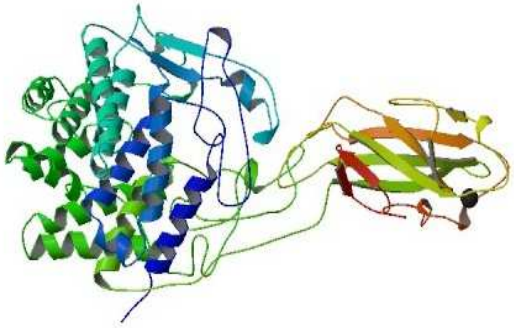
Some bacteria and fungi use this vast resource of carbon in the environment as a nutrient source (Dashtban et al. 2010). Cellulose needs to be broken down into smaller units before it can be used as a nutrient by organisms in the environment. They produce a range of enzymes to digest cellulose and hemi-cellulose to glucose and other sugars. The cellulases are a family of such enzymes that are produced by bacteria and fungi to break down cellulose (Bagyaraj 1993). The hemicellulases are a diverse group of enzymes produced by bacteria and fungi to break down hemicelluloses (Bradner et al. 1999; Shallom and Shoham 2003).

The substances in this group are used industrially in detergents, food, pulp and paper, agriculture, animal feed improvement, and in the bioconversion, textile and fermentation industries (Kuhad et al. 2011; Polizeli et al. 2005). Additionally, all three enzymes in this group have reported uses in hydraulic fracturing as a breaker, which involves reversing crosslinking and thereby reducing the viscosity of gelled fluids in hydraulic fracturing or pre-treatment formulations (European Commission 2002; Stringfellow et al. 2014). Enzymes are highly specific and they usually act under milder reaction conditions than the inorganic chemicals used for this purpose.

All members of this group are continuously discharged into the environment, mainly as a result of their ongoing use in detergents and other domestic situations. There they are susceptible to denaturation and biotic and abiotic degradation (European Commission 2002). Denaturation and loss of function of an enzyme is usually caused by physical effects such as heat, dilution, change in pH, and detergents. Denaturation facilitates the proteolytic

degradation process where proteins can be degraded abiotically by acid catalyzed hydrolysis of peptide bonds (Fugitt 1942) and biotically through enzymatic digestion by proteases (Ramsay and Pullammanappallil 2001). This degradation results in proteins being broken down into their constituent polypeptides and amino acids, followed by further degradation into organic compounds, mostly in the form of short-chain and branched-chain organic acids, ammonia, carbon dioxide, and small amounts of hydrogen and sulfur (Ramsay and Pullammanappallil 2001). These decomposition products can then used by microorganisms as substrate in their anabolic pathways.

23.3 Chemical identity and biological description

CAS Name	**Cellulase**
CAS RN	9012-54-8
AICS name	Cellulase
Enzyme Commission number	EC 3.2.1.4
Synonyms	1,4-β-D-Endoglucanase 1,4-β-D-Glucan 4-glucanohydrolase Various commercial synonyms Bactosol, Endoglucanase, Rucolase
Representative structure[1] endo/exocellulase E4 (*Thermomonospora fusca*) [1]RSCB Protein databank	
Representative molecular weight	95.21 kilodaltons (kDa)
CAS Name	**Hemicellulase**
CAS RN	9025-56-3
AICS name	Hemicellulase
Enzyme Commission number	n/a, member of the EC 3.2.1 group
Representative structure	n/a, group is too large for a representative structure
Synonyms	Various commercial synonyms: Accelerase, Novozyme 348
CAS Name	**CBI (referred to as “enzyme”)**
CAS RN	CBI

23.4 Physico-chemical and biological properties

The standard suite of physical and chemical properties for chemical substances is not relevant for enzymes. They are better defined according to their biological properties and data for one type of enzyme from each enzyme family are presented in **Error! Reference source not found.**.

Type	Cellulase[1]	Xylanase[2]	Enzyme
Name	GH3 β-glucosidase	Endo-1,4-β-D-xylanase	Not presented
Organism	*Myceliophthora thermophila*	*Fusarium heterosporum*	Not presented
pH	3–8	4–6	5-9
Temperature (°C)	50–80	45–60	50-60
Km (substrate)	2.64 mM (cellobiose)	5.26 mg/ml (birchwood)	Not presented
v_{max} (µmole/min/mg)	30.7	800	Not presented
Half life	4.6 h at 50 °C	53 min at 45 °C	80 h at 50 °C
Reaction type	Random hydrolysis of 1,4-β-D-glycosidic linkages	Glycosidase, hydrolyzing O-glycosyl bonds	Not presented
Natural substrate	cellulose, lichenin and cereal β-D-glucans	Various, including xylans, glucans, galactans, mannans, pentosans	Not presented

1. Karnaouri et al. (2013). 2. Heinen (2014).

The properties listed in **Error! Reference source not found.** include the pH range and temperature range where these enzymes are active as well as the reaction type as defined by the nomenclature committee of the International Union of Biochemistry and Molecular Biology (NC-IUBMB). The Michaelis constant (Km) represents the affinity of the substrate for the enzyme. A low Km indicates a high affinity and the maximum rate (v_{max}) of the reaction will be reached more quickly. It is important to note that all three enzyme families, although represented by a single CAS RN, contain a large number of individual enzymes. Theses individual enzymes will have different properties reflecting the biological environment of the organism from which they originate.

23.5 Domestic and international regulatory information

No specific environmental regulatory controls or concerns were identified within Australia and internationally for substances in the Enzymes group.

23.6 Environmental fate summary

The enzymes in this group are produced and destroyed within all terrestrial and aquatic ecosystems (European Commission 2002). They are ubiquitous, naturally occurring proteins which play important roles in the degradation of plant biomass and dissolved organic matter. The environmental fate of the enzymes in this group is expected to be regulated by natural abiotic and biotic degradation processes.

Proteins released into the terrestrial environment will be adsorbed quickly in the soil protecting them from immediate degradation. The persistence and degradation of the proteins in soil both depend largely on microbial activity, which is affected by soil type, pH, temperature, moisture content and other physicochemical and biological characteristics of the soil (APVMA 2011). Proteins can remain in the soil for several weeks, but they are susceptible to desorption and can be washed out by water.

In an aquatic environment the complete hydrolysis of the model protein bovine serum albumin (BSA) can be achieved within 48 hours when exposed to bacterial assemblages (Roth and Harvey, 2006). The bacterial community structure and the respective environment have little effect on the production of protein degradation products (Crottereau 1998; Nunn et al. 2003; Roth and Harvey 2006). Degradation of BSA was found to be different in seawater compared to sediment with sedimentary digestion producing fragments that are larger than those generated in seawater (Nunn et al. 2003).

Few studies are available that investigate the fate of proteins that are released into the environment on an industrial scale. Biodegradation studies with cellulase and the enzyme showed that both enzymes are readily biodegradable under controlled conditions (ECHA 2015). Lipases used in the food and detergent industries have been shown to be readily biodegradable with up to 99% biodegradation after 28 days (Greenough et al. 1996). Proteases used commercially in detergents vary as to the extent they degrade in the environment depending on the test system used (NICNAS 1993; Swisher 1969). However, all proteases analysed were considered readily biodegradable with one report suggesting complete loss of enzymatic activity within 24 hours and full degradation of the enzyme within two days (Swisher 1969).

Based on this information, the enzymes in this group could remain in soil for some time prior to transport within runoff, depending on the microbial activity in the receiving soil. It is expected that they will rapidly denature in the aquatic environment and will be degraded by organisms and extracellular enzymes naturally present in aquatic ecosystems.

23.7 Environmental effects summary

Based on their biological properties and the environmental fate of enzymes generally, especially their relatively short half-lives, prolonged exposure of aquatic organisms to the intact enzymes will be highly unlikely. Extensive toxicological testing of cellulase and the enzyme did not reveal any evidence of acute toxicity of the enzymes (ECHA 2015). With the exception of some sensitising and irritating properties, enzymes used so far do not exhibit toxic or ecotoxic properties that raise significant concern (European Commission 2002).

23.8 Screening assessment

23.8.1 Assessment

The emission of the enzymes in this group from their intended use in hydraulic fracturing can be considered a localised release where the enzyme concentrations in the environment will typically decrease rapidly. Accidental spills of the enzymes could occur during transport. This may result in a release of functioning enzymes directly into the environment. However, the same or homologous enzymes are already present in the environment and pathways exist to degrade them. Additionally, the enzymes have no demonstrated acute toxicity and because of their short lifetime chronic toxic effects are not expected.

The use of the enzymes in this group for applications in coal seam gas extraction is unlikely to cause harm to the environment due to the rapid breakdown of the enzymes and the lack of any significant evidence of toxicity.

23.9 Outcome

A Tier 1 assessment of the environmental risks from the use of substances in the Enzymes group is not required.

23.10 References

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24 Group assessment – Wood products

Not supplied **Wood dust**
Not supplied **Wood fibre**
Not supplied **Walnut hulls**
Not supplied **Nut hulls**
Not supplied **Natural fibres I**
Not supplied **Natural fibres II**
CBI **Natural fibres III**

Confidentiality from public disclosure was claimed for the names and other identifiers of one type of nut hull and two natural fibres. Confidentiality from public disclosure was also claimed for the name and Chemical Abstracts Service Registry Number (CAS RN) of one substance that is also classed as a natural fibre. Information about the identity of these four materials subject to commercial-in-confidence claims was provided to the assessment team and a screening assessment of all four natural materials was conducted. All four materials are referred to as either 'nut hulls' or 'natural fibres' (as appropriate) in the subsequent assessment.

24.1 Grouping rationale

The seven members of this group are all solid materials that are derived from wood or other plant products. Some of these materials do not meet the definition of industrial chemicals as defined under the *Industrial Chemicals (Notification and Assessment) Act 1989*. Nevertheless, all seven materials are composed of similar biopolymers and they have generally similar physical characteristics: they are insoluble plant-derived particles and fibres. The potential environmental concerns of all seven materials are therefore considered sufficiently similar to be assessed together in the same group.

24.2 Background

Wood is a term used to refer to the secondary xylem of woody plants. It is a composite material composed primarily of the three biopolymers: cellulose, hemicellulose, and lignin. Cellulose and hemicellulose comprise 60 to 75% of dry wood and lignin comprises a further 15 to 25%. Cellulose is a high-molecular weight linear homopolymer of glucose which forms long chains that are embedded in a matrix of lignin in the secondary cell walls (Stern et al. 2003). Lignin is a high-molecular weight polyphenol with a complex and variable three-dimensional chemical structure (Chen 2014).

Wood is the most important example of so-called ligno-cellulosic materials. However, there are other important examples of ligno-cellulosic materials from woody plants, including the hulls and shells of single-seeded fruits (drupes) such as walnuts (Stern et al. 2003). The term 'hull' is used to describe the mesocarp of the fruit which surrounds the hard shell (or endocarp), which in turn encases the seed (or kernel) in drupes (Saura-calixto et al. 1983). The hull of walnuts are comprised of a significant proportion of acid-soluble sugars in the form of pectins, whereas the shells have a very low pectin content (Saura-calixto et al. 1983). The shells (endocarp) of drupes such as walnut, peach and coconut are lignin-rich and have a higher proportion of lignin than cellulose (Mendu et al. 2011).

Wood fibre, nut hulls and natural fibres are used for fluid loss control within drilling fluid formulations in the Australian coal seam gas industry. Loss circulation is the result of drilling fluid escaping into the formation by way of crevices or porous media (Bucksch 1997). Nut hulls are also used as a placement aid (a means of controlling formation permeability) and a flow and conductivity enhancer (a means of reducing drag and increasing velocity (Gorse et al. 2012) within hydraulic fracturing or fracturing pretreatment formulations.

The predominant degradation pathway for woody materials in the environment is expected to be microbial decomposition, whereby extracellular enzymes secreted by bacteria and fungi breakdown or otherwise transform the biopolymers in plant cell walls (Blanchette 2000; Pérez et al. 2002; Wetzel 2001). Such decomposition processes are ubiquitous in the environment and are an important part of the biogeochemical carbon cycle.

24.3 Environmental fate summary

Wood and other plant based materials are biodegraded by bacteria and fungi, over sometimes very long (i.e. 1 000 year) time scales, with wood being an important carbon source in terrestrial ecosystems (e.g. Blanchette 2000; Wetzel 2001). The rates of decay and the biochemical pathways involved in wood decay are dependent on the environment in which the wood occurs, with decomposition possible in both anoxic and oxic environments (Pérez et al., 2002; Wetzel 2001).

Vegetation is the primary supplier of organic carbon to the soil (CSIRO Division of Soils 1983), with organic carbon concentrations above 2% preferred for productive agricultural soils (Reid and Dirou 2004). Once in soils, organic carbon plays an essential role in retaining nutrients, soil moisture, improving soil structure, and supplying nutrients (CSIRO Division of Soils 1983; Reid and Dirou 2004).

Organic carbon is also critical to the functioning of aquatic ecosystems, with between 70 and 80% of the organic carbon in aquatic ecosystems in the form of humic and fulvic acids (Wetzel 2001). These acids are produced as a result of the degradation of lignin and cellulose in both oxic and anoxic environments.

The cellulose of wood products is broken down by cellulolytic microorganisms including bacteria, fungi and some anaerobic protozoa and slime (Pérez et al. 2002). In cellulosic wastes, cellulolytic microorganisms can establish synergistic relationships with non-cellulolytic species which result in the complete degradation of cellulose. Under aerobic conditions, carbon dioxide and water are released, whereas carbon dioxide, methane and water are released under anaerobic conditions (Béguin and Aubert 1994; Leschine 1995).

Lignin is primarily broken down by aerobic fungi, first into soluble macromolecules with carboxylic acid and other oxidised functional groups, then into humic and fulvic acids (Wetzel 2001).

24.4 Environmental hazard summary

The materials in this group are transportable into water bodies either through indirect pathways where they can be entrained in runoff, or direct pathways as a result of spillage. The increased turbidity which may result from discharge of materials in the Wood products group into a water body and the decreased transfer of light which would then occur is considered to potentially cause direct non-toxic physico-chemical stress (ANZECC and ARMCANZ 2000).

The dissolved oxygen concentrations in waters receiving wood products could also decrease due to the microbial decomposition of the additional load of organic materials. However, the

magnitude of any such decrease will depend on the rate of decomposition of the additional load of wood products entering the water body compared to the typical background inputs from natural sources (e.g. Wetzel 2001). A decrease in oxygen concentration in the aquatic compartment can also act as an indirect physico-chemical stressor, whereby the behaviour of other physico-chemical stressors is changed as a result of oxygen depletion (ANZECC and ARMCANZ 2000). For example, the oxidation-reduction potential of a water body is expected to decrease with decreased oxygen concentrations (Wetzel 2001). This has the potential to mobilise otherwise insoluble inorganic species such as phosphorous, resulting in blooms of cyanobacteria and consequently lethal depletion of oxygen levels in the water compartment (ANZECC and ARMCANZ 2000).

Woody materials that have not been chemically treated are not considered to be directly toxic to biota. Nevertheless, organic matter such as woody materials can act as non-toxic stressors that have direct or indirect effects on aquatic ecosystems. However, the potential for wood products to act as non-toxic stressors should be considered in context with materials analogous to those in this group expected and sometimes prevalent in most soil and aquatic environments.

24.5 Screening assessment

24.5.1 Assessment

Materials in this group are all derived from wood or other natural plant-based materials and are largely composed of high molecular weight biopolymers such as cellulose, hemi-cellulose, and lignin. Wood products distributed in the terrestrial environment are expected to become part of the organic carbon pool in the soil where it will act as an important physical and chemical constituent. In the aquatic environment, wood products can be viewed as particulate organic matter and are expected to become part of the aquatic carbon cycle. Decay rates for wood products in aquatic ecosystems are highly variable, with woody materials degrading before they reach the sediments in some aquatic ecosystems and being preserved for centuries in others (Wetzel 2001).

Although large quantities of wood products in water could decrease dissolved oxygen concentrations, such impacts are not expected to occur before clean-up or dispersion in receiving waters can occur. Impacts on turbidity could also occur if wood products occur in the form of suspended particulate matter, but these impacts are again expected to be short term due to the settling of wood products from the water column as they become saturated with water.

24.6 Outcome

A Tier 1 assessment of the environmental risks from the use of materials in the Wood products group is not required.

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25 Group assessment – Boron compounds

26038-87-9 Boric acid (H3BO3), compound with 2-aminoethanol
12008-41-2 Boric acid, (H2B8O13), disodium salt
1303-96-4 Borax ((Na2(B4O7).10H2O)

25.1 Grouping rationale

The risk assessment of these three boron compounds has been carried out as a group because regardless of the parent compound the dominant boron species will be the same under normal environmental and physiological conditions (WHO 1998). Furthermore, on a boron equivalent basis the substances in this group are likely to have similar toxicological and chemical properties when dissolved (WHO 1998).

25.2 Background

Boron is naturally present in soil, rocks and water, but is never found as the free element in the environment. Instead, it is always found chemically bound to oxygen in boric acid or as borates – including borax (also known as *tincal* [$Na_2(B_4O_7).10H_2O$]). Boron is an essential micronutrient in plants (Sommer and Lipman 1926). In higher animals and humans, boron has been shown to have beneficial effects, however, its essentiality is still debated (Nielsen 2014).

Boron oxides, boric acid and sodium borates (e.g. borax) have a wide range of applications in industry (e.g. manufacture of glass, fibreglass and porcelain enamels), agriculture (e.g. fertilisers, herbicides and insecticides), and in household settings (e.g. flame retardants and detergents) (Power and Woods 1997). Fibreglass manufacture is the largest single use of boric acid and borates (23%), although significant amounts are also used in detergents (17%) (WHO 1998).

In coal seam gas applications, the hydraulic fracturing fluid primarily consists of sand, water and guar gum. Boric acid or borates such as borax are commonly added to this guar gum slurry to increase its viscosity and provide stability (Stringfellow et al. 2014). The borate ions formed by both substances in water provide cross-links between linear guar gum polymers. After fracturing, enzymes or inorganic substances (termed ‘breakers’) are added to the fracturing fluid to disrupt the guar polymer structure and to break boron cross-links (Stringfellow et al. 2014). All three boron compounds in this group are reported to have uses as cross-linkers or viscosity modifiers in hydraulic fracturing fluids used in Australia.

In the environment, the chemicals in this group will dissociate and/or hydrolyse to release boron as boric acid [$B(OH)_3$ (also formulated as H_3BO_3)] and/or borate anions. Boron naturally enters the environment primarily through processes such as the weathering of rocks and soils, volcanic activity, and the volatilisation of boric acid from sea water (WHO 1998). The majority of boron is found in oceans at concentrations between 0.5 and 9.6 mg of total boron per litre (mg B/L) (Weast 1976). However, the element is ubiquitous in the environment and is found in freshwater and soils at concentrations between <0.01 to 1.5 mg B/L and 1 to 100 mg B/kg, respectively. Globally, soils have an average total boron concentration between 10 and 20 mg/kg (Nable et al. 1997; Power and Woods 1997). In this assessment,

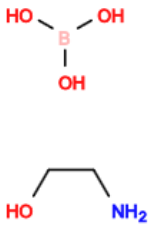
boron concentrations (e.g. mg B/L or mg B/kg) refer to *total* boron concentrations unless otherwise specified.

Dissociation and hydrolysis of the chemicals in this group will also release sodium cations or 2-aminoethanol. Sodium cations have low toxicity at typical environmental concentrations and are naturally ubiquitous in the environment, while 2-aminoethanol has previously been determined to be of low environmental concern (NICNAS 2015). Therefore, the information presented in the following assessment is for the boron species only.

25.3 Chemical name and identification

The monoethanolamine compound with boric acid in this group (CAS RN: 26038-87-9) has indefinite chemical composition. According to industry information, alkanolamine borates such as this substance are complex mixtures of monomeric and polymeric borate esters and salts (Alkanolamine Borates Consortium 2015).

Structural formulae have not been provided for the two sodium polyborate salts in this group. The solid state structure of these salts is typically complex and the structure of the polyborate anions in the solid state does not persist in dilute aqueous solution (Cotton and Wilkinson 1988).

CAS Name	**Boric acid (H_3BO_3), compound with 2-aminoethanol (1:?)**
CAS RN	26038-87-9
AICS name	Boric acid (H_3BO_3), compound with 2-aminoethanol
Synonyms	Monoethanolammonium borate MEA borate Orthoboric acid, compound with 2-aminoethanol
Structural formulae for components	
Formula	$C_2H_7NO \cdot xBH_3O_3$
Molecular weight	Not applicable
SMILES for components	B(O)(O)(O).NCCO

CAS Name	**Boron sodium oxide ($B_8Na_2O_{13}$)**
CAS RN	12008-41-2
AICS name	Boric acid, ($H_2B_8O_{13}$), disodium salt
Synonyms	Disodium octaborate Sodium borate

CAS Name	**Boron sodium oxide ($B_8Na_2O_{13}$)**
Formula	$B_8Na_2O_{13}$
Formula weight	340.46 g/mol

CAS Name	**Borax ($B_4Na_2O_7.10H_2O$)**
CAS RN	1303-96-4
AICS name	Borax (Na2(B4O7).10H2O)
Synonyms	Disodium tetraborate decahydrate Borax Boric acid (H2B4O7), disodium salt decahydrate Tincal
Formula	Na2(B4O7).10H2O (or Na2(B4O5(OH)4.8H2O)
Formula weight	381.37 g/mol

25.4 Physico-chemical properties

Limited measured data are available for the compounds of boric acid in this group. In the environment, these chemicals are expected to dissociate and/or hydrolyse to release boric acid at neutral pH. Therefore, measured data available for boric acid have been presented as analogue data for these substances. This analogue chemical is also expected to be the dominant boron species formed from the dissociation and hydrolysis of borax at environmentally relevant concentrations (Cotton and Wilkinson 1988).

Properties	**Boric acid ($B(OH)_3$) (Analogue)***	**Borax ($Na_2(B_4O_7).10H_2O$)^**
Physical form	White or colourless crystalline granules	White or colourless crystalline granules
Melting point	169°C (decomposition point)	75°C (decomposition point)
Boiling point	Not applicable	Not applicable
Water solubility	63.5 g/L at 20°C	5.92 g/100 g at 20°C
pK_a*	9.14	9.14 (boric acid)
Vapour pressure	Not available	Not available

**(Weast 1976); ^(WHO 1998)*

25.5 Domestic and international regulatory information

25.5.1 Australia

In Australia, high reliability trigger values for boron for freshwater have been determined (ANZECC and ARMCANZ 2000a). The trigger values (**Error! Reference source not found.**) were calculated using four taxonomic groups and are expressed as NOEC equivalents (i.e. chronic end-points were adjusted). Irrigation water trigger values are also given as irrigation

water is a major source of high boron levels in agricultural soils (WHO 1998). Trigger values and guideline values for boron in Australian freshwaters, agricultural waters and agricultural soils are:

Freshwater [#]				**Agricultural irrigation water**[#]		**Agricultural soils***	**Agricultural soils**[&]
Trigger values for a specified level of species protection (mg B/L)^				Trigger value (mg B/L)		Recommended threshold value (mg B/kg) – extractable boron	Upper background value for uncontaminated Australian soils (mean) (mg B/kg) – extractable boron
99%	95%	90%	80%	LTV	STV		
0.090	0.37	0.68	1.3	0.5	NA	15	0.87

LTV = long-term trigger value (up to 100 years use) determined based on crops that are most sensitive to boron; STV = short-term trigger value is not given as it is dependent on crop type (ANZECC and ARMCANZ 2000b).
 # (ANZECC and ARMCANZ 2000a)
** This is not a guideline value, but rather a generally accepted threshold for extractable boron concentrations in agricultural soils (top 100 mm of soil) and exceeding this concentration is likely to cause toxicity to plants (Government of South Australia) and is referenced in (ANZECC and ARMCANZ 2000b)*
^ A trigger value is a concentration that, if exceeded, alerts water managers to a potential change and thus triggers a management response (DPIPWE 2014). The percentage of species to be protected is site-specific (e.g. in an undisturbed ecosystem, 99% of species should be protected).

In Australia, health investigation levels (HILs) have been set for total boron concentrations in soil, and range from 3 000 to 12 000 mg B/kg (standard residential use and residential use with minimal soil access, respectively). However, these levels are not intended to be protective of terrestrial organisms. Although the HILs refer to total boron and not extractable boron, the level is still significantly greater than the threshold for extractable boron in agricultural soils (15 mg B/kg, top 100 mm of soil). It is generally accepted that exceeding this threshold will cause toxicity to plants (Cartwright et al. 1986, Government of South Australia 2009). Other research has suggested that horticultural crops may be more sensitive to boron toxicity. There is insufficient background data to determine a soil cumulative contaminant loading limit (CCL).

25.5.2 European Union

Borax (CAS RN 1303-96-4) has been identified as a Substance of Very High Concern (SVHC) under the European Union Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation due to its reproductive toxicity in humans. It is currently listed on the Candidate List for Authorisation (ECHA 2010). Boric acid, ($H_2B_8O_{13}$), disodium salt (CAS RN 12008-41-2) and boric acid (H_3BO_3), compound with 2-aminoethanol (CAS RN 26038-87-9) have not been identified as SVHCs. However, boric acid (CAS RN 10043-35-3) has been identified as a SVHC and is currently listed on the Candidate List for Authorisation.

25.5.3 Canada

Canadian water quality guidelines (CWQG 2009) have been established for boron for the protection of freshwater organisms following long-term and short-term exposure (1.5 and 29 mg B/L, respectively). A soil quality guideline value for boron in agricultural soils has been set at 2 mg B/kg (CCME 2014). Canadian guideline values have not been set for boron in residential/commercial/industrial soils.

25.6 Environmental fate summary

All of the chemical in this group will transform into boric acid in the aquatic environment. This simple mononuclear boron compound is highly water soluble and is the predominant form of dissolved boron in surface waters. It is a mobile species in the environment and is to be found in all major environmental compartments.

25.6.1 Dissolution and speciation

In the environment, borates and compounds of boric acid will dissociate and/or hydrolyse to form the same boron species (WHO 1998). For example, when borax dissolves in dilute solutions, it dissociates into Na^+ ions and the tetraborate anion ($B_4O_5(OH)_4^{2-}$). Boric acid ($B(OH)_3$) is formed following acid catalysed hydrolysis of the tetraborate anion. Under alkaline conditions, dilute solutions of the tetraborate anion depolymerise rapidly to the mononuclear borate anion ($B(OH)_4^-$) (Cotton and Wilkinson 1988).

Boric acid ($B(OH)_3$) has been used as an analogue chemical in this assessment as this will be the dominant boron species in surface waters under typical environmental conditions. Boric acid is a Lewis acid that acts as a weak monoprotic acid by accepting OH^- and not as a proton donor (pK_a 9.14). Therefore, at the near neutral pH of most environmental systems and at low concentrations (<0.025 mol B/L), the unionised mononuclear species ($B(OH)_3$) will dominate and only a small proportion of boron will exist as the borate monoanion, $B(OH)_4^-$ (WHO 1998).

Polyborate anions (e.g. $B_3O_3(OH)_4^-$ and $B_5O_6(OH_4)^-$) are present in concentrated solutions, however, their concentrations will be negligible in the environment (Ingri et al. 1957).

25.6.2 Partitioning

Boron compounds occur in the atmosphere as particulate matter or as a vapour, with the latter being the dominant form in air. The largest contributor to boron in the atmosphere is volatilisation of boron from seawater. However, boron is not present in the atmosphere at significant levels due to the low volatility and high solubility of borates (Sprague 1972). The average concentration of boron in the atmosphere is low (20 ng/m^3) (WHO 1998).

Boric acid is highly water soluble and it tends to accumulate in surface waters. Although some partitioning from water to soil and sediment does occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5 to 9.0) (WHO 1998).

Borates can adsorb to soil particles. However, under certain conditions, boron is relatively mobile and susceptible to leaching – particularly in acidic, sandy soils that receive high rainfall (Keren and Bingham 1985). Conversely, boron can accumulate in heavy-textured sodic soils that have a high concentration of clay and Al/Fe oxides and receive low rainfall (550 mm/yr). The adsorption of boron to clay particles increases at high ionic strength (Peak et al. 2003). The main factors that control the adsorption of boron to soil particles are soil type, concentration of organic matter, concentration of Al/Fe oxides, clay mineralogy, and soil pH.

Soil pH is one of the most important factors affecting boron adsorption. Over the pH range of 3 to 9, boron adsorption increases with increasing pH. Maximum adsorption usually occurs near the *pKa* of boric acid (9.14) (the affinity of clay minerals for the uncharged boric acid species ($B(OH)_3$) is relatively low). Above this pH, the borate anion ($B(OH)_4^-$) becomes the dominant species and boron adsorption decreases due to competition with OH^- ions for adsorption sites.

The mechanisms that control the adsorption of boron on clays are not fully understood, however it is likely that boron adsorbs to the edges of clay minerals (Goldberg 1997). As boric acid is relatively soluble and mobile in soil, boron usually only accumulates in heavy clay soils in low-rainfall areas.

25.6.3 Bioaccumulation

Boric acid does not accumulate in mammals, fish or insects. However, it does accumulate in aquatic and terrestrial plants, but does not biomagnify through the food chain (Goldberg 1997). The uptake of boron by plants is a passive process (Dannel et al. 2002). Boron is transported from the roots to the shoots in the xylem where it accumulates following evapotranspiration. Once in the leaves it is typically considered immobile as it does not translocate to other plant parts (e.g. fruit). However, recent evidence suggests that in some species, specifically those that transport polyols, boron is mobile in the phloem and can be transported to other plant tissues (e.g. flowers or grain) (Hendrix 2005).

25.6.4 Transport

Boric acid and the borate ion occur naturally in the environment and enter soils and aquatic systems primarily through the weathering of rocks and other geological processes. Although they are highly soluble in water and tend to accumulate in surface waters, they do have the potential to partition to other compartments as discussed above. Under certain conditions, boric acid is relatively mobile in soils and is susceptible to leaching as it is soluble in soil solution.

25.7 Environmental effects summary

In ecotoxicological tests for boron, the exposure concentrations are expressed as boron equivalents i.e. mg B/L. This is because boric acid and borate salts will have the same boron speciation when dissolved in environmental matrices. Therefore, in the following sections toxicological values are given as mg B/L regardless of the form of boron that was tested.

25.7.1 Critical environmental effects

25.7.1.1 Acute toxicity endpoints for aquatic organisms

The following measured median effective concentrations (EC50) and lethal concentrations (LC50) for model organisms were identified for boron (exposure either as boric acid or borax):

Taxon	Endpoint	Method
Fish	96 h LC50 = 332 mg B/L	*Pimephales promelas* (NAPM 1974)
Invertebrates	48 h LC50 = 133 mg B/L	*Daphnia magna* (Gersich 1984)
Algae	72 h EC50 = 34 mg B/L	*Scenedesmus subspicatus* (Guhl 1996) Growth inhibition

There is an extensive set of acute aquatic toxicity data available for boron compounds, including test results for aquatic plants, microalgae, aquatic invertebrates, and fish

(WHO 1998). The weight of evidence from these studies is that soluble boron compounds generally have low to very low toxicity to aquatic organisms in short-term exposures.

25.7.1.2 Chronic toxicity endpoints for aquatic organisms

The following No-Observed-Effect-Concentrations (NOEC) for model organisms were identified for boron:

Taxon	Endpoint	Method
Fish	30 d NOEC = 14 mg B/L 60 d NOEC = 24 mg B/L	*Pimephales promelas* (Butterwick et al. 1989)
Algae	72 h NOEC = 10-24 mg B/L	*Scenedesmus subspicatus* (Guhl 1996)
	8 d NOEC = 20 mg B/L	*Microcystis aeruginosa* (Bringmann and Kuhn 1978)
Bacteria	72 h NOEC = 291 mg B/L	Pseudomonas putida (Schöberl and Huber 1988)

There is an extensive set of chronic aquatic toxicity data available for boron compounds, including tests with a wide range of species in the sensitive early stages of development (WHO 1998). The results of these studies show that boron has generally low toxicity to aquatic organisms in long-term exposures.

25.7.1.3 Toxicity effects on terrestrial organisms

Boric acid and borax have insecticidal, fungicidal and non-selective herbicidal properties. For this reason, boron compounds are commonly used in domestic settings to control pests such as ants, termites and fruit flies. However, these properties typically only present at very high boron concentrations.

Although boron is required by plants at low concentrations, at high concentrations it is toxic. There is only a narrow concentration range where boron is beneficial to the plant; it is in fact the narrowest of all nutrient elements (Goldberg 1997; Peak et al. 2003).

Ecotoxicological tests with plants and soil invertebrates have recorded modest chronic toxicity values (NOECs/EC_{10}'s) in the range of 15.3 to 84.0 and 5.2 to 315 mg total B/kg, respectively (ECHA 2008). However, to predict the potential toxicity of boron to plants and soil organisms, measuring the total boron concentration may be unsuitable. Instead, potential toxicity is better predicted using boron concentrations in the soil solution (extractable boron) (Mertens et al. 2011). In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron (Brennan and Adcock 2004, Government of South Australia 2009).

The phytotoxicity of boron is dependent on the plant species and soil type. Field trials have shown that phytotoxicity may occur if boron concentrations in irrigation water exceed 0.3 to 4 mg/L (Keren and Bingham 1985, Marschner 1995). For example, in an agricultural setting, very sensitive crops cannot tolerate soil water concentrations that are >0.5 mg B/L, whereas very tolerant crops (e.g. asparagus) can tolerate boron concentrations up to 15 mg/L (ANZECC and ARMCANZ 2000b).

Boron toxicity to plants is more likely when it is present closer to the soil surface, where roots encounter high levels of boron in the early stages of development or as seedlings. The

physiological effects of boron toxicity to plants include reduced cell division, decrease in leaf chlorophyll concentrations, and disruption to antioxidation pathways. These effects cause plant stunting and reduced growth (Nable et al. 1997).

25.8 Categorisation and other characteristics of concern

25.8.1 PBT categorisation

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment (UNECE 2007; US EPA 2007).

25.9 Screening assessment

The boron-containing chemicals in this group are expected to have the same speciation when released into the environment, where uncharged boric acid $B(OH)_3$ and the borate mono-anion ($B(OH)_4^-$) will dominate. Borates are widespread, naturally occurring substances in the environment and have low toxicity to aquatic organisms. However, moderate soil concentrations can cause toxic effects in terrestrial plants (phytotoxicity).

Accidental spills of the chemicals in this group will result in the release of boron to the environment. Release to surface waters under these circumstances is expected to have limited long-term environmental effects due to the low chronic aquatic toxicity of boric acid to aquatic organisms. Release to surface soil may result in localised toxic effects in terrestrial plants, depending on background boron concentrations, affected plant species, and soil characteristics. However, spills of large volumes of these chemicals are expected to be cleaned up before extensive uptake of boron by terrestrial plants in the affected area.

Further release of boron to the environment may occur through the use of coal seam gas wastewater for irrigation purposes (Davies et al. 2015). Repeated application of coal seam gas wastewater on heavy textured sodic soils that receive low rainfall (<550 mm/yr) is expected to result in local geoaccumulation of boron. This may cause toxic effects in agricultural crops cultivated on irrigated land, but wider environmental effects are expected to be limited by the low mobility of boron under these conditions. If repeatedly applied to acidic, sandy soils that receive high rainfall (>550 mm/yr), boron present in coal seam gas wastewater is expected to be relatively more mobile. Plant stunting and reduced growth may be experienced in exposed terrestrial plants in the environment as the chemical moves off agricultural lands.

25.10 Outcome

Although the chemicals in the Boron compounds group have generally low aquatic toxicity, they are used in substantial quantities in some hydraulic fracturing operations and they have some phytotoxicity. The large quantities of boron compounds that are used for hydraulic fracturing present a potentially significant point source environmental emission of an element which may accumulate in soil and have phytotoxic effects under certain conditions.

The potential for accumulation of boron in soil from beneficial reuse of wastewater from coal seam gas operations in activities such as dust suppression and irrigation is a specific risk factor for this group of chemicals, which may be more significant in areas with sodic alkaline soils.

25.11 References

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26 Polyesters

26.1 Background

Polyesters are polymers typically formed by condensation of polyhydric alcohols and polybasic acids (Sharp 1990). They are produced on a large scale for industrial applications, but they also occur as natural products (e.g., Spring 1945). Polyethylene terephthalate (PET) is the most common type of synthetic polyester. It is typically produced as a very high molecular weight plastic polymer material that is widely used in fibres, bottles and packaging (US NLM 2015). Other common polyesters include those used in biodegradable plastics (Fakirov 2015).

Polyesters are reported to be used in the coal seam gas industry in Australia in drilling fluid formulations as bridging agents. According to industry information, bridging agents are solids which are used to plug fractured or porous rock formations in order to prevent fluid loss during drilling operations. The loss of fluid into formations during drilling results in a reduction or loss of fluids returning to the surface in a process which is referred to as lost circulation. When bridging agents are used to manage lost circulation they are referred to as lost circulation materials (LCMs). The chemical composition of LCMs is variable, but they are typically readily available solid materials which have fibrous or plate-like forms (Almargo and Frates 2014; Schlumberger 2016).

The specific chemical identities of the polyesters used as bridging agents were not available for this assessment. However, the available information suggests that polyester LCMs are likely to be made from PET. This abundant solid plastic material has high mechanical strength and is thermally and chemically stable. Although it is possible that other types of polyester may be used in LCMs, it is reasonable to assume that any such products will also be made from high molecular weight polyesters that are chemically and thermally stable. This assessment has therefore been conducted on the basis that the polyesters used as bridging agents in the domestic coal seam gas industry are stable and insoluble PET particles, flakes and fibres.

26.2 Environmental fate summary

Polyethylene terephthalate (PET) is very stable in the natural environment due to the aromatic sub-units of its polymeric structure. These protect the ester bonds from cleavage by microbial enzymes and from hydrolytic cleavage by abiotic processes. Thus, under normal environmental conditions, PET is almost impervious to hydrolytic degradation and is essentially a non-biodegradable solid (Ivanova 2013).

The main mode of degradation of PET plastics in the environment is photodegradation (Ivanova 2013). The exposure of PET to near ultraviolet light results in cleavage of the ester links in the polymer backbone by processes which include radical reactions and inter- and intra-molecular hydrogen shifts. As photodegradation proceeds, the bulk material becomes brittle, crazed and discoloured (Venkatachalam 2012). After extensive exposure to light the bulk material will begin to disintegrate and the component polymer chains will eventually reach a sufficiently low molecular weight that they can be metabolised by microorganisms. The rate of degradation is very slow and strongly dependent on exposure conditions (e.g., exposure to UV light). It has recently been estimated that it can take 50 years or more for PET to fully degrade in the environment (Ivanova 2013).

26.3 Environmental effects summary

Synthetic polymers that are stable in the environment, that have high molecular weight and low charge density, and that do not swell in water generally pose a low risk of causing direct ecotoxicological effects in the environment. For polyesters with these properties, adverse effects are typically only expected to occur in the environment as a result of physical effects, such as the blocking of respiratory organs (Boethling and Nabholz 1997).

Polyesters may pose an ecotoxicity concern if they are water soluble or dispersible and they have high cationic charge density. Water soluble cationic polymers have the potential to adsorb to anionic biological membranes of aquatic organisms, which can cause various toxic effects (Boethling and Nabholz 1997). Polyesters that rapidly degrade into low molecular weight species may also pose a concern as low molecular weight degradants are generally more bioavailable than the parent polymers. If degradation of such polyesters results in release of chemical species that are persistent, bioaccumulative, and toxic (PBT), they may be considered of high concern to the environment. Polyethylene terephthalate does not present any of these hazards.

26.4 Screening assessment

26.4.1 Assessment

Polyethylene terephthalate is a very high molecular weight plastic material with very low bioavailability and high stability in the environment. It belongs to a class of ubiquitous industrial plastic materials that are generally considered to have very low potential for direct ecotoxicity.

In common with other stable synthetic plastics, PET does have some potential to present various physical hazards to the environment due to its slow degradation. However, significant release of PET particles, flakes and fibres into surface waters and soil from their down-hole use as a lost circulation material is not expected. Furthermore, any accidental spills of these inert plastic materials could be easily managed by standard spill control measures and the recovered material could be re-used, or safely disposed of to landfill.

26.5 Outcome

A Tier 1 assessment of the environmental risks from the use of polyethylene terephthalate (PET) as a lost circulation material is not required.

26.6 References

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