

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

*Technical report number 9*

## **Environmental exposure conceptualisation: Surface to surface water pathways**

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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## Citation

This report should be cited as:

Department of the Environment and Energy 2017, *Environmental exposure conceptualisation: Surface to surface water pathways*, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy, as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia project, Commonwealth of Australia, Canberra.

## Acknowledgements

This report is one in a series prepared under the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia. It was prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy.

The report's authors gratefully acknowledge input from the Project Steering Committee, which comprised representatives from the National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the Department of the Environment and Energy, the CSIRO, Geoscience Australia (GA), and an independent scientific member, Dr David Jones of DR Jones Environmental Excellence.

This report was subject to internal review and independent, external peer review by staff of the US EPA and by Emeritus Professor John Chapman. Their input is gratefully acknowledged.

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Technical report number	Title	Authoring agency
<b><i>Reviewing existing literature</i></b>		
1	Literature review: Summary report	NICNAS
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
<b><i>Identifying chemicals used in coal seam gas extraction</i></b>		
7	Identification of chemicals associated with coal seam gas extraction in Australia	NICNAS
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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
<b><i>Assessing risks to workers and the public</i></b>		

Technical report number	Title	Authoring agency
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
<b><i>Assessing risks to the environment</i></b>		
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<sup>1</sup> 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 Independent Expert Scientific Committee on Coal Seam Gas and Large Coal Mining

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<sup>1</sup> See Mallants et al. 2017a; Jeffrey et al. 2017; Adgate et al. 2014; Flewelling and Sharma 2014; DEHP 2014a; 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.

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.

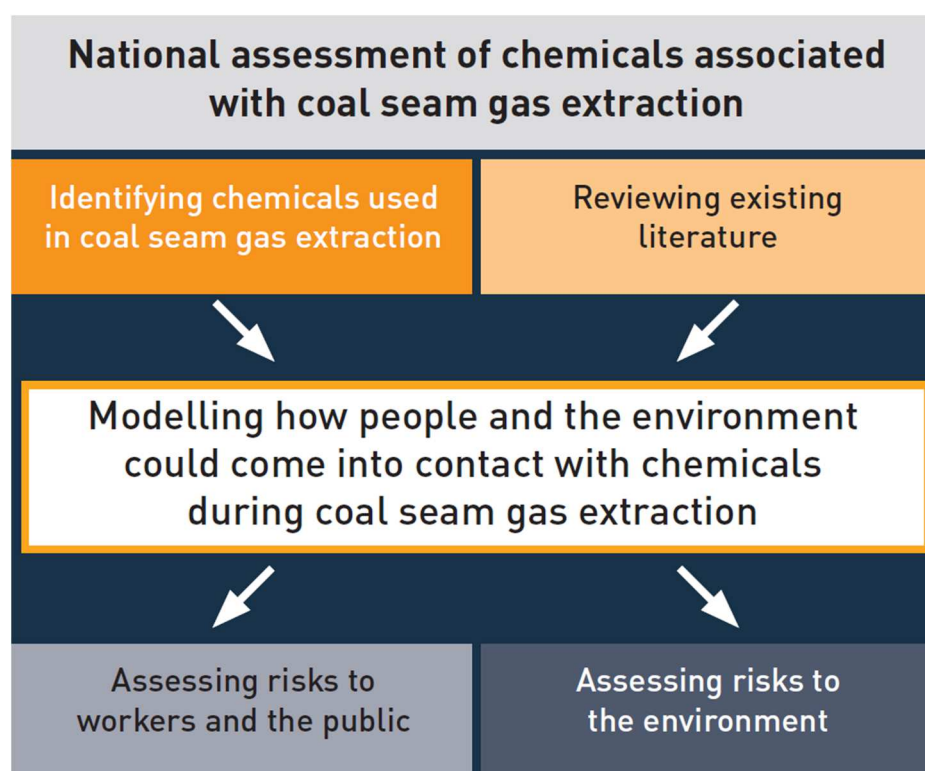


Figure F.1 Steps in the assessment

## 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 exposure conceptualisation: Surface to surface water pathways***

This report is part of the 'modelling how people and the environment could come into contact with chemicals during coal seam gas extraction' stage of the Assessment. It describes the conceptual models developed for predicting chemical concentrations – that is, hydraulic fracturing and drilling chemicals associated with coal seam gas extraction in Australia – in surface water systems such as wetlands and streams, resulting from spills and leaks at the land surface. These models incorporate the best current understanding of the complex soil and surface water systems to ensure that all of the relevant processes and pathways are included in the subsequently developed predictive numerical models, which will be used to undertake the human health risk assessments.

This report focuses on conceptualisation of surface exposure pathways for chemicals, specifically surface runoff and inputs to surface streams from shallow groundwater. Infiltration and volatilisation are examined as a mechanism for losses from the surface soil and water compartments. The extent of exposure of surface receptors to the shallow groundwater compartment has been considered separately and reported in CSIRO's report *Human and environmental conceptualisations: Soil to groundwater pathways* (Mallants et al. 2017b).

This report describes the lifecycle of chemicals associated with Australian coal seam gas extraction activities, the potential sources of environmental releases on the surface, and the receiving environments and relevant receptors. It also addresses the primary chemical fate pathways for surface releases, and includes consideration of secondary surface exposures resulting from interaction of shallow groundwater with the surface environment. This report is informed by previous literature reviews (DoEE 2017a; Mallants et al. 2017; NICNAS 2017a) and publicly accessible scientific literature.

An important part of the conceptualisation process is to develop the mathematical expressions that will relate the chemical quantities, the points of release and the transfer pathways to the final concentrations that will be seen by the environmental receptors. This work also introduced the three-tiered approach for modelling and the risk assessment that will be followed for the subsequent risk assessment. The general methodologies used to derive the inputs needed for the mathematical relationships are also outlined. These input values (chemical identities, compositions and concentrations in release media) were obtained from literature reviews (DoEE 2017a and Mallants et al. 2017), and from the report *Identification of chemicals associated with coal seam gas extraction in Australia* (NICNAS 2017b). Finally, this report also provides a generic description of the approach to be followed for model validation in the subsequent risk assessment work.

Drawing on the information collated in the previously conducted literature reviews (NICNAS 2017a; DoEE 2017a; Mallants et al. 2017a; Apte et al. 2017a), and the report on the identification of chemicals associated with coal seam gas (NICNAS 2017b), the conceptualisation presented here will directly inform the next stage (risk characterisation) for both the human health and environmental risk assessment processes in the National Coal Seam Gas Chemicals Assessment.



# Abbreviations

General abbreviations	Description
APVMA	Australian Pesticides and Veterinary Medicines Authority
BTEX	Benzene, Toluene, Ethyl benzene, Xylenes
CAS RN	Chemical Abstracts Service Registration Number (a unique identifying number assigned to each chemical)
CBAS	Chemicals and Biotechnology Assessment Section (formerly Chemicals Assessment Section) in the Chemicals and Waste Branch of the Department of the Environment
CBI	Confidential business information
CN	Curve number
CSIRO	Commonwealth Scientific and Industrial Research Organisation
DoEE	Department of the Environment
DSEWPaC	Department of Sustainability, Environment, Water, Population and Communities (now Department of the Environment)
EPBC Act	<i>Environment Protection and Biodiversity Conservation Act 1999 (Cwth)</i>
GA	Geoscience Australia
GIS	Geographical information system
HDPE	High density polyethylene
IESC	Independent Expert Scientific Committee on Coal Seam Gas and Large Coal Mining Development
ML	Megalitre
MNES	Matters of National Environmental Significance
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NSW	New South Wales
OC	Organic carbon
PEC	Predicted environmental concentration
QSAR	Quantitative structure activity relationship (model)
US EPA	United States Environmental Protection Agency

# Glossary

Term	Description
Bioregion	A geographic land area within which coal seam gas and / or coal mining developments are, or could, take place, which will be subject of a bioregional assessment
Bounding estimate	A bounding estimate captures the highest possible exposure, or theoretical upper bound, for a given exposure pathway
Coal seam	Coal seams or coal deposits are layers containing coal (sedimentary rock). Coal seams store both water and gas. Coal seams generally contain more salty groundwater than aquifers that are used for drinking water or agriculture
Coal seam gas	A form of natural gas (generally 95–97% pure methane, CH <sub>4</sub> ) typically extracted from permeable coal seams at depths of 300 to 1 000 m. Also called coal seam methane (CSM) or coalbed methane (CBM)
Conservative approach / assessment	An assessment aimed at deliberately overestimating the potential risks to humans and the environment (after US EPA 1992)
Drilling fluids	Fluids that are pumped down the wellbore to lubricate the drill bit, carry rock cuttings back up to the surface, control pressure and for other specific purposes. Also known as drilling muds
Drilling / Fracturing products	Proprietary mixtures of chemicals – often with a trade name – used by companies to assist in the drilling and / or hydraulic fracturing processes
Edge of field	A point at the edge of a coal seam gas well field that is adjacent to a water body
Environmental compartment	Distinct components of the environment – principally, the atmosphere, freshwater and marine aquatic systems, suspended and bottom sediments, terrestrial soils and terrestrial and aquatic biota
Flowback water	The initial flow of water returned to a well after fracture stimulation and prior to production
Geogenic chemical	A naturally occurring chemical originating from geological formations
Henry's Law	A law stating that the mass of a dissolved gas in a given volume of solvent at equilibrium is proportional to the partial pressure of the gas
Hydraulic fracturing	Also known as 'fracking', 'fraccing' or 'fracture stimulation', is one process by which hydrocarbon (oil and gas) bearing geological formations are 'stimulated' to enhance the flow of hydrocarbons and other fluids towards the well. In most cases is only undertaken where the permeability of the formation is initially insufficient to support sustained flow of gas. The process involves the injection of fluids, gas, proppant and other additives under high pressure into a geological formation to create a conductive fracture. The fracture extends from the well into the coal reservoir, creating a large surface area through which gas and water are produced and then transported to the well via the conductive propped fracture channel
Hydraulic fracturing fluid	A fluid injected into a well under pressure to create or expand fractures in a target geological formation (to enhance production of natural gas

Term	Description
	and / or oil). It consists of a primary carrier fluid (usually water or gel based), a proppant and one or more additional chemicals to modify the fluid properties
Injection	The injection of liquid (e.g. H <sub>2</sub> O) or gas (e.g. CO <sub>2</sub> ) into an aquifer. Commonly used in Managed Aquifer Recharge schemes or groundwater remediation
Mass balance	Identification of mass flow by accounting for material entering and leaving a system
Model validation	The process of determining the degree to which a model or simulation is an accurate representation of the real world from the perspective of the intended uses of the model or simulation
Produced water	Water that is pumped out of coal seams to release natural gas during the production phase. Some of this water is returned fracturing fluid and some is natural 'formation water' (often salty water that is naturally present in the coal seam). This produced water moves through the coal formation to the well along with the gas, and is pumped out via the wellhead
Proppant	A component of the hydraulic fracturing fluid system comprised of sand, ceramics or other granular material that 'prop' open fractures to prevent them from closing when the injection is stopped
Risk assessment	A process to estimate the risk of an adverse effect to a given target organism, system, or (sub)population, including the identification of attendant uncertainties, following exposure to a particular agent, taking into account the inherent characteristics of the agent of concern as well as the characteristics of the specific target
Stream order	Stream order is a measure of the relative size of a stream, being dependent upon the arrangement of converging stream branches. For example, a second-order stream is formed when two first-order streams converge
Toxicity	Inherent property of an agent to cause an adverse biological effect
Unsaturated zone	Also known as the 'vadose zone'. This zone extends from the top of the ground surface to the water table, where the soil pores are at atmospheric pressure

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# 1 Introduction

## 1.1. Environmental exposure conceptualisation

This report outlines the exposure scenarios (i.e. release points and transfer pathways) and mathematical expressions used in the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, particularly the environmental risk assessment (DoEE 2017b) and to assist with the human health risk assessment (NICNAS 2017c).

The four key stages of the chemical lifecycle that were considered for their potential release of chemicals into the environment are identified in Section 2. These stages are transport, storage, industrial use, and disposal. The important features of each of these stages are discussed, as are chemical fate pathways and the receiving environments that they provide the source terms for. The environmental exposure scenarios investigated do not extend to the contamination of animal or plant-based food produce as no data were available on the levels of chemical residues in food linked to contamination by drilling and hydraulic fracturing operations. These systems also do not form part of the natural ecosystem under study and thus were outside of the scope of the environmental risk assessment.

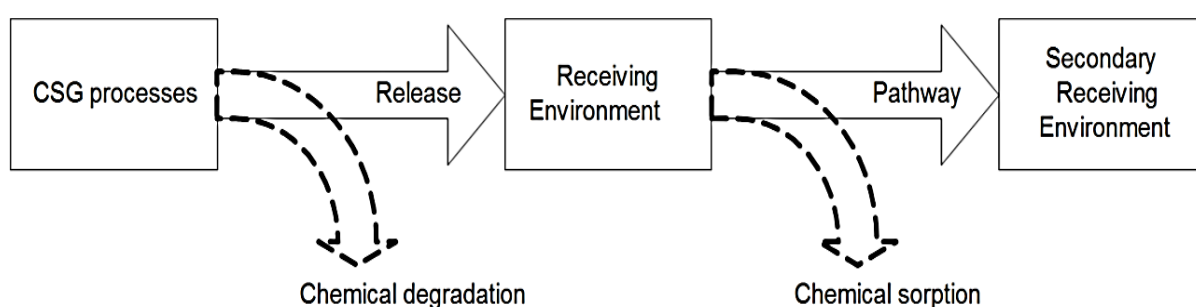
Following identification of the most likely exposure scenarios, Sections 3 and 4 describe the mathematical expressions (and required input data) for predicting the quantities of chemicals released, and their concentrations in the receiving surface environments. This report also provides a generic description of the tiered approach to be followed in the subsequent risk assessment.

Section 5 outlines the approach for model validation to be used for the subsequent risk assessment. A summary of the equations and approaches discussed in this report is provided in Section 6.

## 2 Exposure scenarios

### 2.1. Introduction

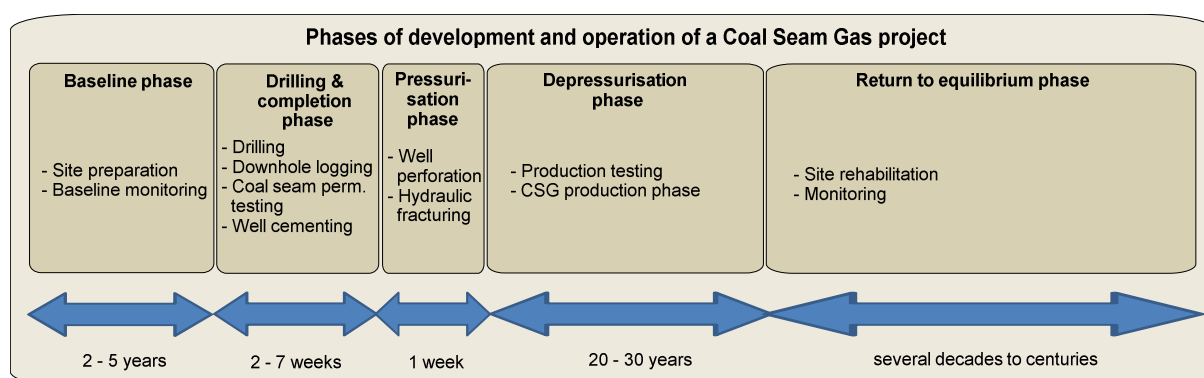
This section establishes how potential environmental exposure, and subsequent human exposure, may occur as a result of coal seam gas extraction in Australia. It describes the lifecycle of chemicals associated with Australian coal seam gas extraction activities, potential sources of environmental release, the receiving environment, and chemical fate pathways which may result in loss of chemicals (e.g. through dilution, degradation, and / or sorption processes) or subsequent exposure in a secondary receiving environment. Figure 2.1 shows, in a simplified form, how these elements are interrelated in the conceptualisation of environmental exposure adopted in this report.



Note: CSG = coal seam gas.

Figure 2.1 Conceptualisation of environmental exposure

The lifetime of an individual coal seam gas well or an entire coal seam gas well field can be divided into different phases (Figure 2.2). Each phase involves distinct activities with a relatively well defined duration and set of risks. Importantly, these risks are not equally distributed across time and space.



Source: Mallants et al. (2017b)

Figure 2.2 Phases of development and operation of a coal seam gas project with typical activities. Duration of each phase is indicative (length of arrows is not to scale)



The phases of development and operation of a coal seam gas well field are as follows:

1. *Baseline or pre-development phase*: starts when the site is being established and includes activities such as site identification, site access and preparation, baseline monitoring prior to production well construction. This may take between two to five years.
2. *Drilling and completion phase*: includes activities such as well construction starting with a bare site, building a pad and pond, setting up the rig, drilling, installing casing and piping, and cementing. This is followed by pump installation, completion of the surface gathering system, and connecting the well to the gathering system. The duration of the phase is normally from two to seven weeks.
3. *Pressurisation or hydraulic fracturing fluid injection phase*: starts with the first injection of hydraulic fracturing fluid into the coal formation and terminates when the last fluid is injected. There may be a number of injection events in the life-time of the site. The duration of the injection phase is from hours to days. It should be noted that the majority of production wells in Queensland and New South Wales have not required hydraulic fracturing because the permeability is sufficiently high for gas to flow due to natural fractures. Companies are preferentially targeting these areas initially. Coal seams in the Bowen Basin (Queensland) have a much lower permeability than the Surat Basin (Queensland), and as a result, hydraulic fracturing will likely have greater application in the Bowen Basin than in the Surat.
4. *De-pressurisation phase*: starts soon after hydraulic fracturing phase ends, and covers both flowback and production, including the extraction of gas and water from the coal seam until gas and water extraction ends. In a coal seam gas well, water flow rates are initially high with low gas flow rates but as the coal seam formation is progressively de-pressurised, gas flow rates continue to rise to a peak rate, months or years after de-watering started, and water flow rates decline. There may be a number of de-pressurisation events intermittent with injection phases. The total duration of the de-pressurisation phase may be up to 20 and 30 years.
5. *Return to equilibrium or post-operational phase*: starts at the end of the de-pressurisation phase and finishes when groundwater pressures have been restored to their pre-operational levels. It includes activities such as decommissioning, plugging, rehabilitation, and monitoring. This is done progressively as wells are depleted, plugged, and abandoned. The cessation of water extraction via a coal seam gas well does not necessarily result in an overall restoration of the original groundwater pressures. It will depend, among other things, on how fast groundwater can flow towards the zones that experienced de-pressurisation. In other words, although the de-pressurisation phase has ended because water extraction has stopped, it may still take a very long time to restore all groundwater pressures to the pre-operational conditions. Duration of the post-operational phase can be in excess of 100 years.

Potential sources of surface-related contamination have been reviewed and are reported in Apte et al. (2017), DoEE (2017a), Jeffrey et al. (2017), NICNAS (2017a), and Mallants et al. (2017a). Additional information about potential sources of contamination and their release are reported in NICNAS (2017b). Potential risks of contamination of soil and groundwater from chemical use associated within each of the different phases involved in developing a coal seam gas well field have been summarised by CSIRO (Mallants et al. 2017a) and are further conceptualised by Mallants et al. (2017b). The following discussion focuses on potential releases of chemicals used or produced during the pressurisation / injection, de-pressurisation, and return to equilibrium phases.

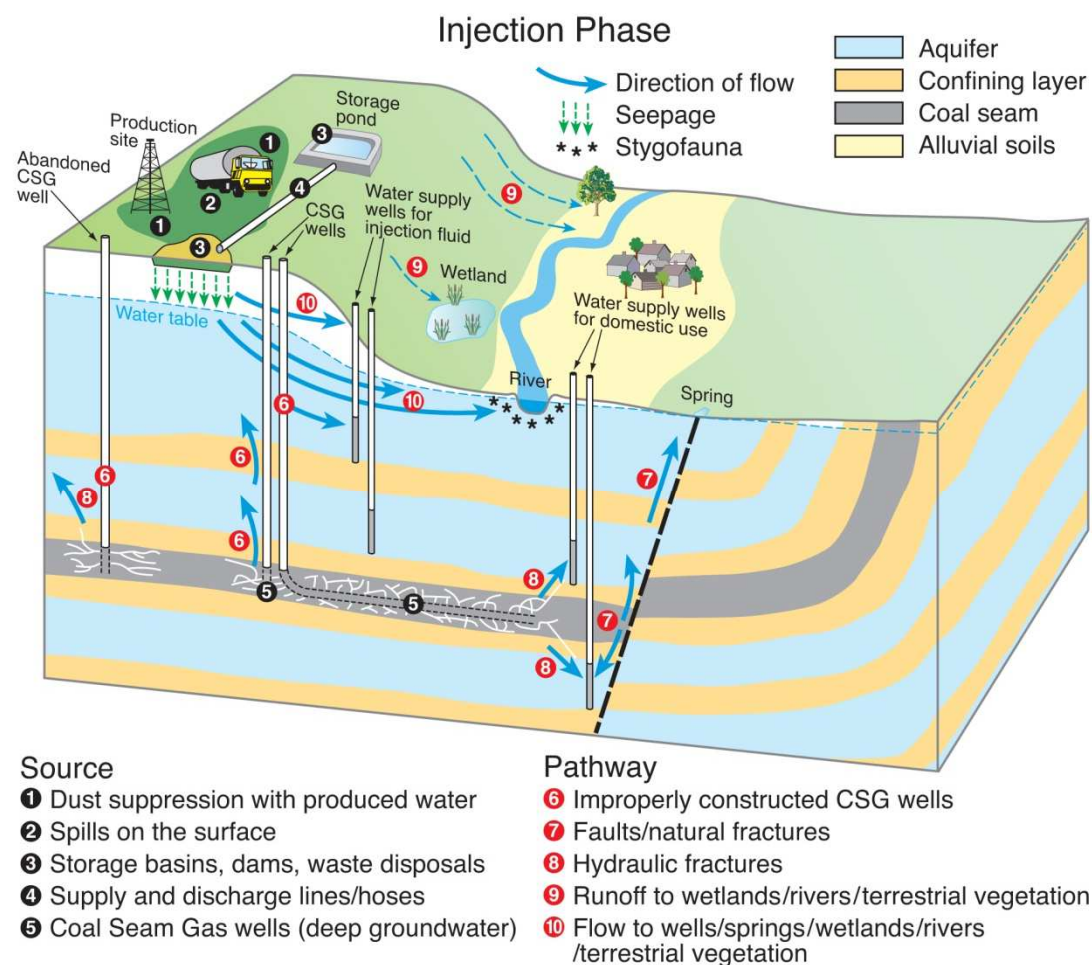
As part of the consideration of environmental impacts associated with coal seam gas operations within the pressurisation, de-pressurisation, and return to equilibrium phases, there is potential for contamination of surface waters, soil, and shallow groundwater by fluids

associated with storage, transport, mixing, injection, surface spills, surface handling of drilling and hydraulic fracturing chemicals and other fluids associated with coal seam gas extraction (i.e. flowback water and produced water). This can result from:

- spill or leaks
- leakage from storage impoundments
- improperly constructed well casings
- poor recovery of fluids injected during the hydraulic fracturing process
- intentional surface applications of treated or untreated produced water for beneficial use (see 'Sources' in Figure 2.3 for pressurisation phase and Figure 2.4 for de-pressurisation phase).

During the de-pressurisation or production phase, water and gas are mostly separated within the coal seam gas well. In each coal seam gas well water is pumped up through the tubing, and gas flows up the annulus (the space between the casing and tubing). The water from the coal seams is pumped to storage ponds awaiting treatment and / or re-use. Assessments of possible contamination pathways from surface spills through soil and groundwater to receiving environments (such as rivers, water wells, wetlands, and springs) during the production phase requires consideration of the following potential sources of contamination (Figure 2.4):

- *Infiltration of flowback and produced water into soil due to use of this water for dust suppression at a site* (Source 1 in Figure 2.3 and Figure 2.5). Dust generation at the site and on access roads will need to be controlled which typically requires regular water spraying. This water is generally treated, to varying degrees.
- *Infiltration from incidental spills on the surface from storage tanks, trucks, valves, etc.* (Source 1 in Figure 2.3 and Figure 2.5). Spills may be contained and managed through on-site spill containment processes. Depending on the volume of water released and antecedent soil moisture conditions (e.g. from rainfall), potential contamination may be limited to the soil zone and never reach the groundwater table. Risks for groundwater contamination will be higher for shallower soil in combination with larger release volumes.
- *Infiltration from storage basins or waste disposal ponds; dam wall collapse; hazardous events including flooding* (Source 3 in Figure 2.3). In Australia design requirements for storage basins include the bottom of the basins being sealed with a clay liner or a material with an equivalent low permeability (e.g. high density polyethylene (HDPE) plastic sheet). Nevertheless, some leakage is considered likely, based on manufacturing specifications.
- *Releases from supply and discharge lines and hoses that transport produced water from the well site to the storage ponds* (Source 4 in Figure 2.3 and Figure 2.5). Leaks from subsurface discharge lines carrying produced water to a storage pond may potentially occur as a result of construction faults, destruction of pipelines due to road works or land preparation works, etc.



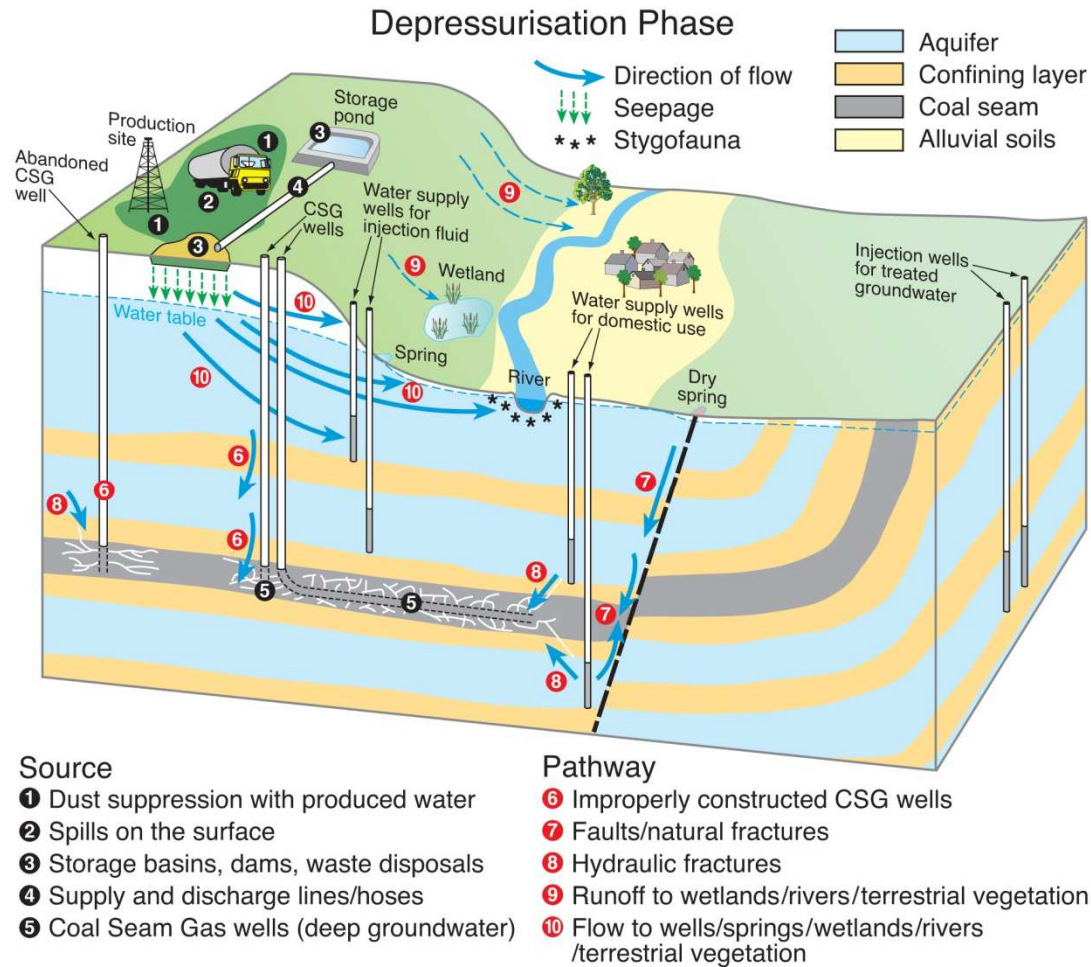
Source: Mallants et al. (2017b)

Figure 2.3 Possible contaminant sources at the coal seam gas site (1 to 5) and pathways for solute transport during the injection of hydraulic fracturing fluids – injection or pressurisation phase (6 to 10)

Assessments of possible contamination pathways from surface sources to surface receiving environments (such as rivers, wetlands, etc.) during the drilling, pressurisation (Figure 2.3 and de-pressurisation phases Figure 2.4) requires consideration of the following:

- *Runoff to wetlands and rivers* (Figure 2.5) – this includes the potential flow of spilt chemicals on the land surface to water courses [for assessments at the land surface see DoEE (2017a)].
- *Subsurface flow from surface sources to wells, springs, wetlands, and rivers* – the potential flow includes unsaturated zone flow and saturated zone flow, and surface sources (1 to 4), as discussed above.

Discussions about the potential pathways for solute transport in deeper groundwater (pathways 6, 7, and 8 in Figure 2.3) and their potential impacts are beyond the scope of this Assessment. A discussion about hydraulic fracturing in Australian coal seams and likely scenarios for fracturing fluids entering into an aquifer is provided by CSIRO (Mallants et al. 2017a, Jeffrey et al. 2017, and Mallants et al. 2017c).

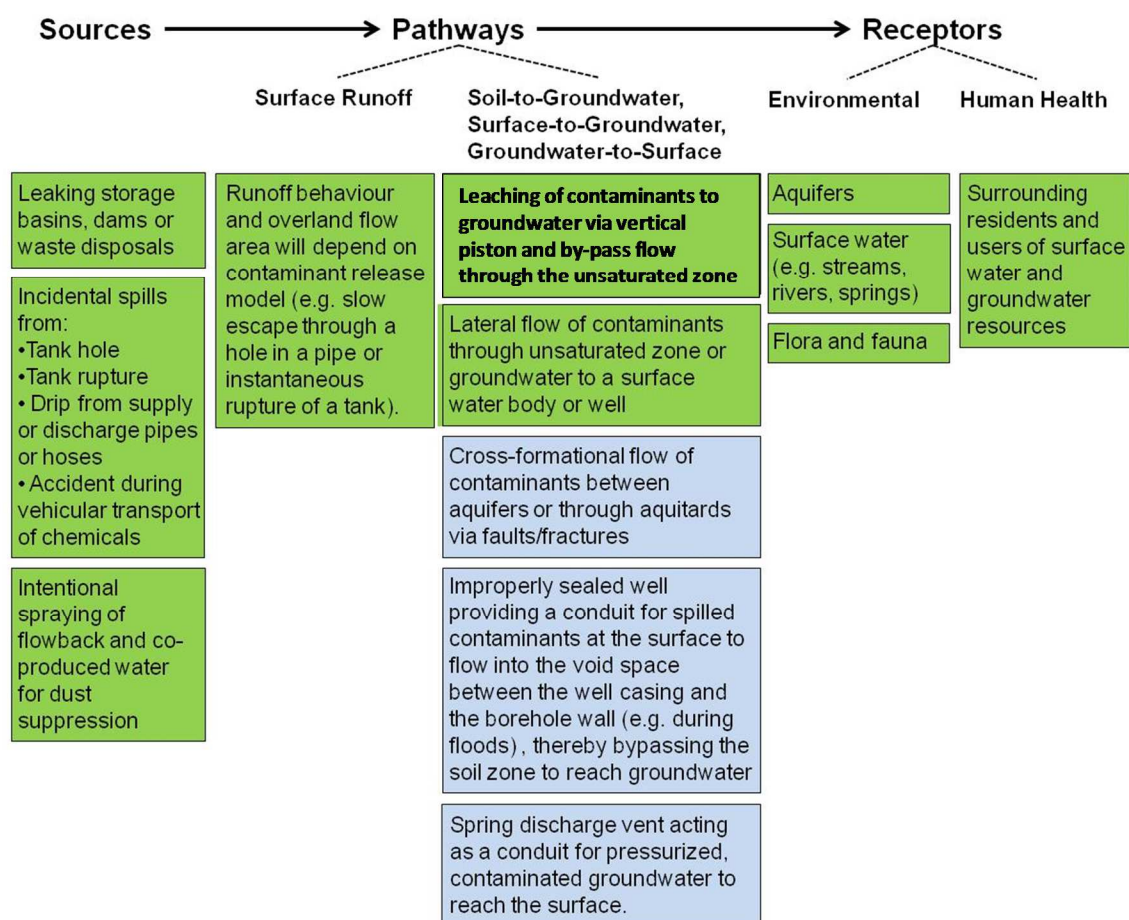


Source: Mallants et al. (2017b)

Figure 2.4 Possible contaminant sources at the coal seam gas site (1 to 5) and pathways for solute transport during the de-pressurisation phase (6 to 10). Source 5 and pathways 6 to 8 are not considered for shallow groundwater assessments

The source of contamination may be due to either a leak from a specified storage unit (e.g. basin, dam, waste disposal pond) or an incidental spill. An additional pathway exists when an improperly sealed well allows spilled contaminants to bypass the soil and unsaturated zone and directly contact groundwater via the void space between the casing and borehole wall.





Note. Boxes shaded in green are within the scope of this study, whereas the boxes shaded in blue refer to deep groundwater and are out of scope.

Figure 2.5 Source-pathway-receptor analysis for contamination derived from spills and leaks

## 2.2. Chemical lifecycle

The environmental exposure assessments conducted as part of the National Coal Seam Gas Chemicals Assessment consider the transport, storage, industrial use, and disposal stages of chemical use. This section of the conceptualisation report provides a process description of each stage of the lifecycle for drilling and hydraulic fracturing chemicals. The coal seam gas process description, as depicted in Figure 2.6, is derived from the information collected in the literature review (DoEE 2017a) and from the report on identification of chemicals associated with coal seam gas extraction completed under the National Assessment (NICNAS 2017b).

### 2.2.1. Transport

Transport of industrial chemicals for use in coal seam gas extraction occurs between the place of import or manufacture and intermediate storage sites, and subsequently to individual well sites. Based on the existing infrastructure in coal seam gas tenements, it is assumed that these industrial chemicals are carried predominantly on trucks rather than by other modes of transport such as rail. It is also assumed that chemicals will be transported in

individual containers on trucks as there was no evidence from the industry survey (NICNAS 2017b) that transport of chemicals occurred by bulk tanker.

Coal seam gas waste products (e.g. used drilling fluids, flowback water, and in limited cases produced water) containing both industrial and geogenic chemicals may be transported by truck or tanker from the well site to storage sites, approved facilities for disposal or alternative locations for re-use, including for re-use in coal seam gas operations. Transport of chemicals in flowback and produced water from well sites to centralised water management facilities is more likely to occur through underground gathering pipes within established coal seam gas tenements.

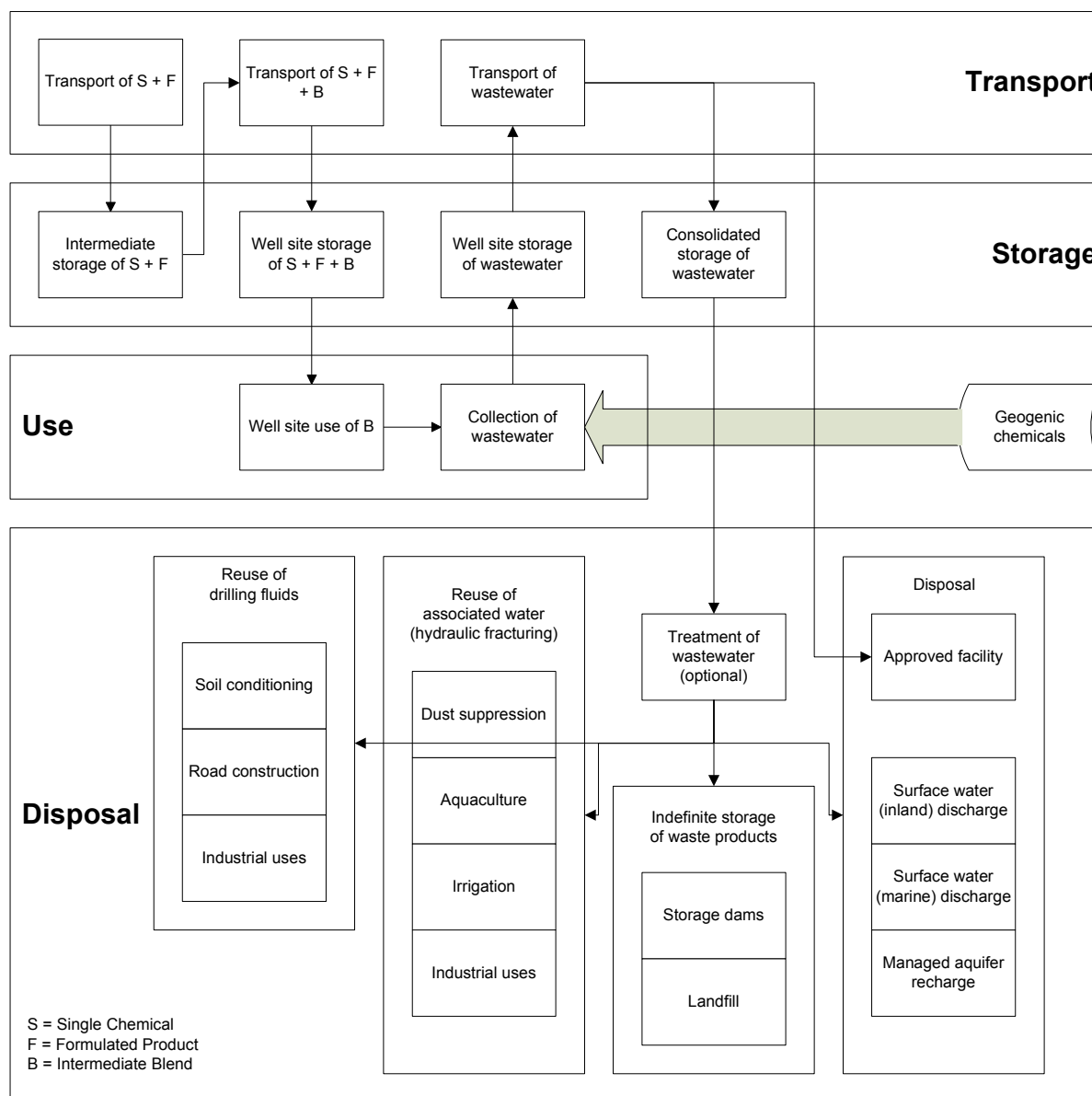


Figure 2.6 Lifecycle stages of chemicals associated with coal seam gas extraction

### 2.2.2. Storage

Industrial chemicals may be stored at an intermediate storage facility at or near a coal seam gas tenement. Such a facility, such as the dangerous good storage area shown in Figure 2.7 would likely hold chemicals for use at several well sites. Industrial chemicals are likely to be

stored at individual well sites for a short time before use in drilling or hydraulic fracturing operations.

Used drilling fluids, flowback water, and produced water may be temporarily stored at individual well sites in tanks or dams. These coal seam gas waste products may also be collected and stored in dams at centralised facilities on or near the tenement prior to treatment and / or re-use. Although evaporation dams are an option of last resort for the long-term management of coal seam gas water, and not recommended, some coal seam gas waste products (including brine) may be stored indefinitely until suitable methods of disposal or re-use are identified.



Source: © DoEE, courtesy B Gray and Origin Energy Ltd.

Figure 2.7 A dangerous goods storage facility housing chemicals associated with coal seam gas extraction

### **2.2.3. Industrial use**

There are some differences between the preparation of drilling and hydraulic fracturing fluids for use. The industry survey (NICNAS 2017b) reports that drilling chemicals are initially blended at intermediate storage facilities. These intermediate blends are typically incorporated into an emulsion consisting of base oil, water and other products at the well site, which is then dissolved within the drilling fluid system. In contrast, hydraulic fracturing chemicals are blended via batch or continuous mixing at the well site.

The transfer of drilling and hydraulic fracturing chemicals to blending units and of the resulting process fluids to the wellhead occurs through a network of temporary, above ground pipes. At the wellhead, process fluids are injected into the subsurface during drilling or hydraulic fracturing operations.

After operations, drilling and hydraulic fracturing fluids are returned to the surface. Returned drilling fluids may be separated from the cuttings on site prior to disposal. Following hydraulic fracturing operations, the well bore is flushed with water and a proportion of the individual industrial chemicals along with geogenic chemicals are expected to be returned to the surface in the flowback water. After use, geogenic chemicals combine with the industrial chemical lifecycle and share the fate of coal seam gas waste products. Geogenic chemicals are expected to be brought to the surface in flowback water and then produced water over the life of the well.

#### **2.2.4. Disposal**

The disposal of coal seam gas waste products containing chemicals involves different options. For example, returned drilling fluid may be re-used if it is synthetic or oil based, while water based drilling fluid is disposed of in accordance with local requirements (DoEE 2017a). Flowback water containing hydraulic fracturing chemicals may or may not be treated (depending on composition) prior to re-use or disposal.

Treatment options for flowback and produced water in the US typically include combinations of the processes and technologies below, depending on the composition of the water to be treated (DoEE 2017a):

- Membrane-based processes including nano-filtration and reverse osmosis
- distillation technology
- filtration
- aeration and sedimentation
- biological treatment
- demineralisation (ion exchange)
- thermal distillation
- condensation
- ionisation
- natural evaporation
- freeze / thaw
- crystallisation and ozonation.

Treatment of flowback and produced water involving removal of chemicals is typically limited to reverse osmosis in Australia. Reverse osmosis treatment results in concentration of the chemicals in the waste stream (i.e. brine). Disposal options for waste concentrates include indefinite storage (e.g. lined ponds), injection into aquifers, and landfill (of solids).

The efficiency of removal of some chemicals may be poor and they could remain in the treated water at concentrations that exceed water quality guidelines (DoEE 2017a). In this case, or where flowback and produced water is not treated, these residual chemicals will follow the re-use or disposal pathway for this wastewater.

Disposal and re-use options for untreated (dependent on composition) or treated flowback and produced water may include:



- send to sewer treatment plant
- aquaculture (with subsequent disposal expected either directly to surface water bodies or re-use in irrigation)
- irrigation of forestry, fuel and food crops
- dust suppression on site (i.e. roads and well pads)
- supplementation of environmental flows through direct discharge to surface water bodies
- injection into aquifers
- indefinite storage (of chemicals) in evaporation ponds.

## 2.3. Points of release

Release to the environment may occur during any of the chemical lifecycle stages. This section describes potential pathways for release to occur, and the controls that are used by industry to minimise release to the environment. The points and mechanisms of release and any control measures are summarised in Table 2.1 and Table 2.2. Mathematical expressions to estimate the release quantity during each stage of the chemical lifecycle are detailed in Section 3.5, while preliminary inputs to use in these calculations are detailed in Section 4.2. Releases may be accidental or intentional.

Table 2.1 Storage release details

Release point	Release mechanism	Control measure
Container	Spill due to piercing	Spill kit, bunding
Blending unit	Spill	Spill kit, bunding
Dam	Wall failure	State dam construction guidelines
Dam	Overflow	State dam construction guidelines
Dam	Leak through dam floor	Lining

Table 2.2 Use release details

Release point	Release mechanism	Control measure
Pipes	Leaks	Spill kit, bunding
Blending unit	Spill	Spill kit, bunding
Wellhead	Blowout	Blowout preventer

### 2.3.1. Transport accidents

Truck accidents may occur at any point along a transport route to intermediate holding warehouses, individual well sites or re-use and disposal sites, potentially releasing single chemicals, chemical formulations or other coal seam gas waste products to the environment. Depending on the location of an accident, release may be direct to an aquatic receiving environment or indirectly from an accident occurring at some distance from an aquatic ecosystem (e.g. a lake or other wetland, stream, or river). In this latter case, release is direct

to soil and subject to runoff and other fate pathways discussed in Section 2.4. Truck accidents are single events where the potential release at any location is limited to the carrying capacity of the truck.

Control measures may contain the contents of a spill or reduce the quantity of chemical entering a pathway to an aquatic receiving environment. These include materials that contain the spillages and spill kits on trucks.

### **2.3.2. Storage accidents**

Mishandling of containers stored at intermediate holding warehouses and individual wells may result in container failure and release to the environment of single chemicals or formulated products. Noting that some chemicals are reformulated, spills of intermediate blends may also occur on site. Examples of mishandling include accidental piercing of containers and spills during reformulation.

The release to the environment of process fluids stored in lined formulation pits prior to their use, or of stored coal seam gas waste products, may arise due to dam wall failure, overflow of dams during rainfall events, and from leaks through the dam lining or floor.

Any potential release of stored single chemicals, formulated products, intermediate blends, and coal seam gas waste products will initially be to soil. Exposure to surface water is expected to result from indirect pathways (e.g. through overland flow) as discussed in Section 2.4. Where included in the site design, spillages that occur during storage may be isolated and contained through spill containment infrastructure and / or by bunding constructed around the chemical storage area. It is also expected that sites will have spill kits for cleaning up spilled chemicals and formulated products. Control measures also apply to dams, which are expected to be constructed with structural integrity and containment features in accordance with state guidelines. Many dams are also lined with HDPE to minimise leaks and chemical exchange with groundwater in accordance with design, construction, and / or manufacturing specifications.

### **2.3.3. Industrial use accidents**

Mishandling accidents at the well site during use may release single chemicals or formulated products to the environment through spills from blending units, leaks from above-ground pipes and from well blowouts. Where blended fluids are stored in lined formulation pits prior to use, rainfall may result in overflow and release to soil. A proportion of blended fluids injected underground during coal seam gas extraction activities may be retained and transported within the subsurface rather than being completely recovered in the flowback water. Recoveries of 52% to 61% of the total fluids injected have been reported based on samples collected over 5 to 19 days, respectively (DoEE 2017a).

With the exception of subsurface release, releases will be initially to soil and any releases to water are expected to be indirect via the pathways discussed in Section 2.4. Spillages during use may be isolated and contained by bunding where this has been included in the site design as it should be. It is also expected that sites will have spill kits for cleaning up spilled chemicals and formulated products, and that blowout preventers will be included in wellheads to minimise the risk of release of any well fluids to the environment (DEEDI 2011).

The intentional release of coal seam gas waste products and brine during disposal is discussed in Section 2.2.4, while accidental release during transport and storage is covered in Sections 2.3.1 and 2.3.2 [further discussion is presented in DoEE (2017a)]. For accidental releases, the spill kits used for the clean-up will be disposed of in landfill.

The information provided in Sections 2.2 and 2.3 is summarised in Table 6.1.

## **2.4. Chemical fate pathways**

This section outlines chemical fate pathways, which may result in the transfer of contaminants between different environmental compartments or the transformation of the chemical through degradation processes. Figure 2.8 illustrates how the fate pathways discussed in this section can lead to chemical movement through the environment. Depending on the physical properties of the chemical, other fate pathways such as volatilisation may need to be included in more detailed quantitative mass balance calculations.

Runoff may occur during a high intensity rainfall event, or series of events, resulting in the transport of contaminants in the soil compartment to a secondary site in the soil compartment or into an aquatic compartment. For example, contaminants released to soil as a result of a container spill may move through a catchment in solution or adsorbed to sediment. The proportion of contaminant in the soil available for runoff is dependent on competing fate mechanisms such as partitioning into the solid phase (adsorption) and degradation as described in Section 3.4.2.

### **2.4.1. Airborne deposition**

Airborne deposition occurs when contaminants in the soil compartment become airborne in dust (as particulates) and are transported through the air before settling at a secondary site. This transport mechanism is driven by wind and may result in exposure to the aquatic compartment. An example of when deposition may be a relevant secondary exposure pathway is when untreated or partially treated flowback or produced water is re-used and applied to soils at well sites or transport corridors for dust suppression. The extent of deposition depends on several factors as described in Section 3.4.3, but is expected to be small compared to the secondary exposure potential of runoff.

### **2.4.2. Partitioning and sedimentation**

Flowback and produced water intentionally released to aquatic ecosystems may contain chemical contaminants, as described in DoEE (2017a). These contaminants may have an affinity for particulates in the water and sediment at the bottom of the aquatic ecosystem. A chemical may adsorb directly to the sediment. Otherwise, it may first adsorb to suspended particles in water, then settle to the sediment. The physico-chemical properties of the chemical and the turbidity (a measure of the concentration of suspended particles in solution) of the water will determine whether the predominant pathway involves direct partitioning to sediment, or settling to sediment over time. This is discussed further in Section 3.4.5.

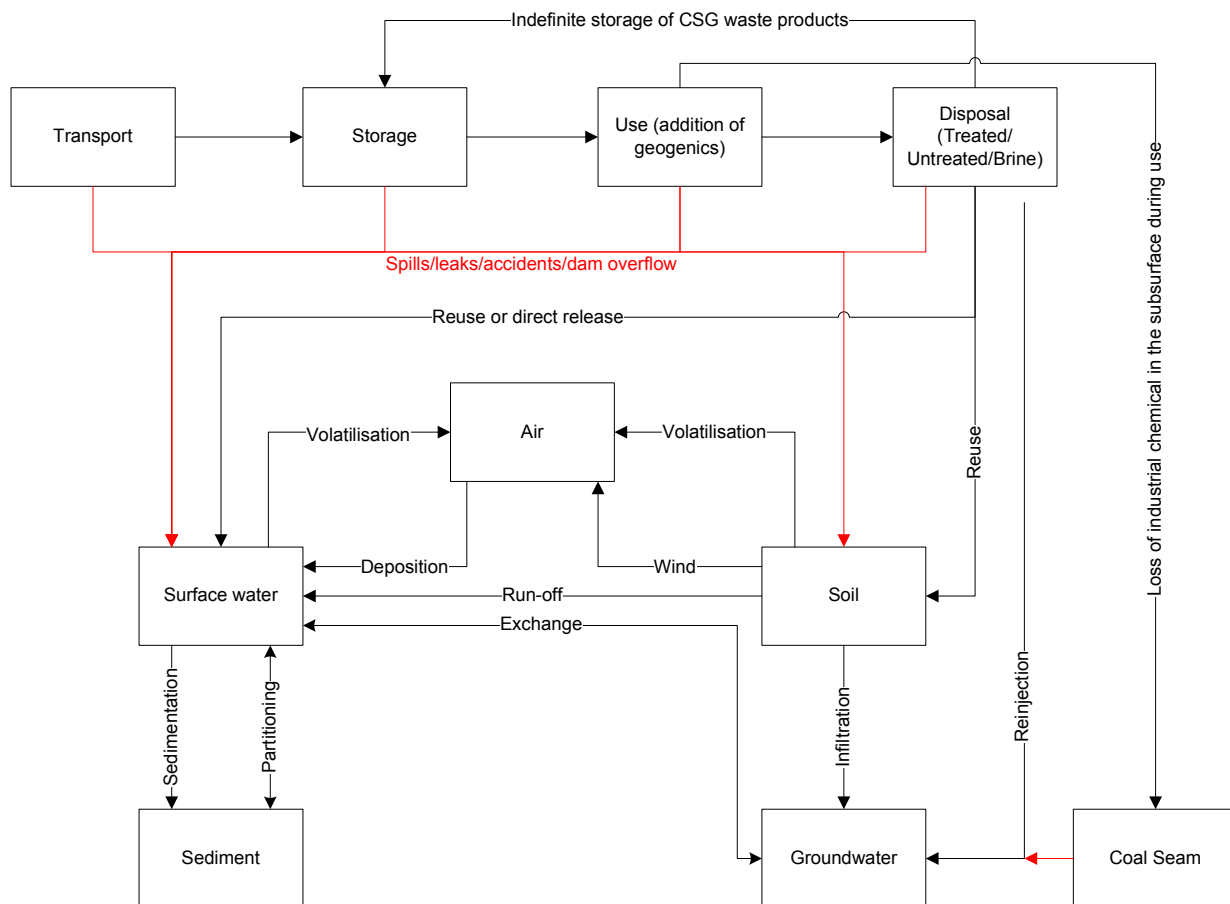


Figure 2.8 Simplified fate pathways for chemicals associated with coal seam gas extraction (red lines show unintended releases)

### 2.4.3. Volatilisation

Volatilisation may occur when contaminants partition to air from the surface of water bodies in which contaminants are present, such as storage dams holding wastewater and drilling fluids or rivers. The likelihood and extent of a chemical volatilising from water is determined by individual chemical properties and environmental factors as discussed in Section 3.4.4. Volatilisation can also occur from soil, for instance after a spill.

### 2.4.4. Degradation

Degradation results in the removal of a contaminant from a compartment through transformation. Transformation can occur in storage ponds or elsewhere in aquatic and soil compartments via various mechanisms including biodegradation and processes such as photolysis and hydrolysis. The approaches for estimating chemical degradation are discussed in Section 3.4.6.

### 2.4.5. Infiltration

Infiltration occurs when contaminants in soil, for instance from a spillage, leach through the soil profile towards groundwater. This may also arise from storage dam leaks. The scope of this report is limited to surface-to-surface exposure. Infiltration is only cursorily examined as a mechanism for losses from the soil compartment. The extent of exposure to the shallow groundwater compartment is not considered in this report, but is considered separately in *Human and environmental exposure conceptualisation: Soil to groundwater pathways*

(Mallants et al. 2017b) and the literature review, *Leakage to shallow groundwater of fluids associated with hydraulic fracturing for coal seam gas extraction* (Mallants et al. 2017a).

## **2.5. Receiving environment**

The receiving environment comprises a range of environmental compartments (such as soil, surface water, and air) into which a chemical may be released, as described in Section 2.3, or into which a chemical may enter (including sediment and groundwater). Each of the environmental compartments considered in this report is briefly described below. Groundwater is not discussed as the scope of this report is limited to consideration of surface-to-surface exposure scenarios. Shallow groundwater exposure is considered in a separate report (Mallants et al. 2017b).

### **2.5.1. Soil**

There are several exposure scenarios which may result in contamination of soil. The intentional release of treated or untreated flowback or produced water may be to agricultural land. Dust suppression using flowback and produced water may be to roads or coal seam gas sites. Spills from transport accidents or mishandling of chemicals may result in contamination of coal seam gas work sites or roads, or adjacent native pasture. Due to different land use and soil types, the soil environment will differ. This may affect the depth to which contaminants penetrate, the area over which they spread and their concentration in soil. It may also affect the contaminants' subsequent transport to other environmental compartments. These influences are described further in Section 3.3.2.

### **2.5.2. Surface water**

The aquatic ecosystem to which contaminants may be released will vary in size and flow rate. The aquatic ecosystem size is expected to be highly variable depending on the location of the release. This variability is treated by considering a hypothetical small aquatic ecosystem, which may exist near the release, and then considering larger water bodies based on actual measured environmental flow. Where a release is considered to occur over a fixed timeframe, then the flow rate multiplied by that fixed timeframe is equivalent to the volume of the aquatic ecosystem. This is further discussed in Section 3.3.1.

### **2.5.3. Sediment**

Chemicals released to water bodies may be adsorb to sediment, which can vary in composition and depth. However, where there is insufficient information to infer sediment depth and composition, default values will be assumed. See Section 3.4.5 for further details.

### **2.5.4. Air**

Air is a dynamic environmental compartment and complexities arising from this are not considered in the simplified approaches used in this report. Instead, the air is assumed to be a homogeneous medium in which emissions are diluted (see Section 3.3.2).

The information provided in Sections 2.4 and 2.5 is summarised in

Table 6.2.

## 3 Mathematical expressions

### 3.1. Introduction

An environmental exposure assessment includes an estimation of release, consideration of environmental fate and partitioning behaviour, and the derivation of predicted environmental concentrations (PEC). Section 2 describes the potential exposure scenarios, how release of chemicals from coal seam gas extraction activities may result in contamination of soil, surface water, air, sediment, and groundwater compartments. This section outlines the mathematical expressions that may be used to quantify chemical concentrations in the receiving environment following release. The scope of this report will be restricted to surface-to-surface exposure, and will therefore not include groundwater.

The scenarios under which chemicals may be released to surficial environments by coal seam gas activities in Australia were investigated using a tiered process consistent with the US EPA Framework for ecological risk assessment (US EPA 2014). The three tiers used to assess chemical release scenarios in this environmental assessment are:

- Tier 1 uses simple models and equations to represent Australia-wide conditions and to calculate PECs. The inputs to the models include readily available standard values, bounding estimate values, assumptions and point estimates.
- Tier 2 includes more detailed modelling to represent bioregional conditions and more complex equations for calculation of PECs. The inputs include real data for the bioregion, high-end estimate values, assumptions and point estimates.
- Tier 3 includes complex and detailed modelling, to represent working site conditions in the bioregion and for the determination of PECs. The inputs include site-specific data, typical or average values for the site or closely related sites, realistic assumptions, and point estimates.

### 3.2. Predicted environmental concentrations

In the simplest terms, the predicted environmental concentration, or PEC, is calculated using Equation 1:

$$PEC = \frac{Q}{V} \quad \text{[Equation 1]}$$

Where:

$Q$  = the quantity of a chemical released into the environment

$V$  = the volume of the receiving environment medium.

This is a simplification of the actual concentration, as it assumes instantaneous mixing and is only representative of the PEC at an instant in time without allowing for changes in the environment. The amount of chemical may change over time due to the addition from further releases to the environment. It may also decrease due to degradation (biotic and abiotic) and transport to other environmental compartments including to air by volatilisation and sediment by partitioning (see Section 2.4). It may also be transported from the initial receiving environment to a secondary receiving environment. This change in quantity of chemical may be represented by  $\Delta Q$ .

Similarly, the volume of the receiving environment may change from additional inflows of rainfall, uncontaminated runoff water and stream flows and dispersion into the wider environment. This change in volume of receiving environment may be represented by  $\Delta V$ . This is discussed in more detail in Section 4.3.1.

Therefore, over time the environmental concentration may be considered using Equation 2:

$$PEC = \frac{Q_i \pm \Delta Q}{V_i \pm \Delta V} \quad [\text{Equation 2}]$$

The values of  $\Delta Q$  and  $\Delta V$  generally will require detailed knowledge of the chemical's fate and transport properties and of the characteristics of the receiving environment. These may not be readily available and therefore will generally not be able to be included in the bounding estimate scenario of a Tier 1 assessment. This issue may be addressed by considering bounding estimate values for  $Q_i$  (quantity of chemical released) assuming that no increase or dissipation is likely to occur, such that  $\Delta Q = 0$ . Similarly, if bounding estimate volumes are chosen for  $V_i$  (volume of the environment) any refinement of  $\Delta V$  will result in a dilution and hence lower PECs. This may be expressed mathematically as outlined in Equation 3:

$$PEC_{\text{bounding estimate}} = \frac{Q_i \text{ bounding estimate}}{V_i \text{ bounding estimate}} > \frac{Q_i \pm \Delta Q}{V_i \pm \Delta V} \quad [\text{Equation 3}]$$

For the sake of simplicity, equations relating to PEC in Tier 1 will be presented in the form of Equation 1. At higher tiers of assessment the more complex form in Equation 2 may be introduced and PEC may be considered as  $PEC_{\text{refined}}$ .

However, by definition:

$$PEC_{\text{upper bound estimate}} \geq PEC_{\text{refined}} \quad [\text{Equation 4}]$$

such that Equation 4 may be expressed as:

$$PEC_{\text{upper bound estimate}} \geq PEC_{\text{refined}} = \frac{Q_i \pm \Delta Q}{V_i \pm \Delta V} \quad [\text{Equation 5}]$$

Since  $\Delta Q$  and  $\Delta V$  can only have positive values (no negative mass or volume), to satisfy the above equation, only a decrease in the quantity of chemical,  $\Delta Q$  (e.g. from degradation) or increase in volume  $\Delta V$  (e.g. an influx of uncontaminated water) will be considered in the refinement of the PEC. This may be expressed as presented in Equation 6:

$$PEC_{\text{refined}} = \frac{Q_i - \Delta Q}{V_i + \Delta V} \quad [\text{Equation 6}]$$

There is an exception to this approach, where there are repeated or continuous releases of a chemical. In this case, the quantity is always changing due to more chemical being introduced such that  $\Delta Q$  is significant when compared with  $Q_i$  and Equation 3 is no longer valid. Similarly, as more chemical is added to a receiving environment it may contaminate a greater volume of water than initially considered. It is therefore not realistic to assume a static environment.

In a system where there is a constant rate of introduction of a chemical and a constant rate of removal of a chemical, these two competing mechanisms will eventually reach equilibrium. This equilibrium is known as the steady-state. The steady-state concentration of a chemical may be calculated according to Equation 7 [adapted from Atkins (1986)]:

$$PEC = \frac{Q \times k_i}{V \times k_r} \quad [\text{Equation 7}]$$

Where:

PEC	= Predicted environmental concentration (kg or L/m <sup>3</sup> )
Q	= Quantity of the chemical in (L or kg)
$k_i$	= Rate constant for introduction (d <sup>-1</sup> )
V	= Volume of the receiving environment (m <sup>3</sup> )
$k_r$	= Rate constant for removal (d <sup>-1</sup> )

In Equation 7, the numerator ( $Q \times k_i$ ) gives a rate of introduction and the denominator ( $V \times k_r$ ) gives the rate of removal.

Where there is repeated release this will result in accumulation of the contaminant in the receiving environment. The accumulation in soil of a contaminant is dependent on the interval at which it is applied and the rate of the contaminant's degradation. The relationship between the initial concentration (PEC<sub>0</sub>) and the final concentration (PEC), when the interval between applications is constant, is expressed based on first order kinetics (Lin et al. 1971) and is mathematically equivalent to the "saw tooth" analysis provided in EPHC (2009b). The relationship between PEC<sub>0</sub> and PEC is presented in Equation 8:

$$PEC/PEC_0 = e^{-kt} \times \frac{\exp[(N+1)kt_b] - 1}{\exp(kt_b) - 1} \quad [\text{Equation 8}]$$

Equation 8 may be rearranged as presented in Equation 9:

$$PEC/PEC_0 = e^{-k(t-Nt_b)} \times \frac{1 - \exp[-(N+1)kt_b]}{1 - \exp(-kt_b)} \quad [\text{Equation 9}]$$

For a bounding estimate analysis only, the maximum concentration (immediately after an application) needs to be considered, such that  $t$  will always be a multiple of  $t_b$ , according to the number of applications ( $t = Nt_b$ ). Accordingly for PEC<sub>max</sub>/PEC,  $t - Nt_b = 0$  and  $e^{-k(t-Nt_b)} = 1$  and Equation 9 can be simplified as presented in Equation 10:

$$PEC_{max}/PEC_0 = \frac{1 - \exp[-(N+1)kt_b]}{1 - \exp(-kt_b)} \quad [\text{Equation 10}]$$

Where the number of applications is indeterminate, a theoretical maximum may be calculated by finding the limit of Equation 9 as  $N$  approaches infinity. Since  $1 - \exp[-(N+1)kt_b]$  approaches 1 as  $N$  approaches infinity, the relationship between PEC<sub>max</sub> and PEC may be represented as shown in Equation 11:

$$\lim_{N \rightarrow \infty} PEC_{max}/PEC_0 = \frac{1}{[1 - \exp(-kt_b)]} \quad [\text{Equation 11}]$$

The variables used in Equation 9, Equation 10, and Equation 11 are shown in Table 3.1.

Table 3.1 Variables used in Equation 9, Equation 10, and Equation 11

Variable	Definition
PEC	Final predicted environmental concentration
PEC <sub>0</sub>	Initial predicted environmental concentration
$N$	Number of applications
$t_b$	Time between applications



Variable	Definition
$t$	Time from first application
$k$	Rate constant for the degradation of the chemical

Many biotic and abiotic processes in environmental compartments such as soil effectively follow single first order kinetics, in spite of their behaviour being controlled by several competing first order kinetic processes (FOCUS 2006). However, the degradation of some chemicals does not follow first order kinetics and this model may not adequately describe accumulation in soil in these cases. Further research is required to determine the relevance of these issues to coal seam gas chemicals in Australia.

### 3.3. Calculating the PEC in the receiving environment

The receiving environment and its volume will intrinsically affect the PEC (by the process of dilution) and therefore elucidation of this volume is an integral part of the PEC modelling process. The quantity of chemical released ( $Q$ ) will also affect the PEC, and is discussed separately in Section 3.5.

The initial receiving environment may be surface water, soil or air. The following section will discuss the modelling of the PEC in these compartments, while Section 3.4 will address the fate of chemicals and their potential to migrate to a secondary receiving environment.

#### 3.3.1. Aquatic PECs

The calculation of the PEC in the aquatic compartment ( $PEC_{\text{aquatic}}$ ) may consider simple dilution of a chemical in an aquatic ecosystem as described generally in Exposure Equation 1. This is appropriate for modelling the PEC from a one-off release event into an aquatic ecosystem occurring over a short period of time (or pulse release) such as a spill.

$$PEC_{\text{aquatic}} = \frac{Q}{V_{\text{water}}} \times 10^6 \text{ mg/L} \quad [\text{Exposure Equation 1}]$$

Where:

$PEC_{\text{aquatic}}$  = Predicted environmental concentration in the aquatic compartment (mg/L)

$Q$  = Chemical quantity loaded to the aquatic ecosystem and / or watercourse (kg)

$V_{\text{water}}$  = Volumetric of the aquatic ecosystem and / or watercourse (L)

The US Environmental Protection Agency (US EPA 2005a and 2005b) developed an equation for the aquatic compartment for calculating a steady-state PEC, with the equation presented in Exposure Equation 2:

$$PEC_{\text{aquatic}} = \frac{Q \times k_i}{V f_x \cdot f_{wc} + k_{wt} \cdot A_w \cdot (d_{wc} + d_{bs})} \quad [\text{Exposure Equation 2}]$$

Where:

$PEC_{\text{aquatic}}$  = Predicted environmental concentration in the aquatic compartment ( $\text{kg/m}^3 \equiv \text{mg/L}$ )

$Q \times k_i$  = Chemical quantity loaded to the aquatic ecosystem and / or watercourse over a period of time (L or kg/d)

$V_{f_x}$	= Average volumetric flow through the aquatic ecosystem and / or watercourse (L/d)
$f_{wc}$	= Fraction of the chemical in the water column (i.e. aqueous component only)
$k_{wt}$	= Overall total aquatic ecosystem and / or watercourse dissipation rate for the chemical ( $d^{-1}$ )
$A_w$	= Surface area of the aquatic ecosystem and / or watercourse ( $m^2$ )
$d_{wc}$	= Depth of water column (m)
$d_{bs}$	= Depth of the upper benthic sediment layer (m)

To calculate the volume of water ( $V_{water}$ ) a sum of the environmental volume ( $V_{environmental}$ , see Section 3.3.1.1), the volume of contaminated water ( $V_{contaminated}$ , see Section 3.3.1.2) and the volume of uncontaminated water ( $V_{uncontaminated}$ , see Section 3.3.1.3) entering the receiving environment as a result of the exposure event needs to be considered. This is represented in Exposure Equation 3:

$$V_{water} = V_{environmental} + V_{contaminated} + V_{uncontaminated}$$

[Exposure Equation 3]

The variables used in Exposure Equation 3 are shown in Table 3.2.

Table 3.2 Inputs for variables used in Equation 3 at each Tier

Variable	Tier 1	Tier 2	Tier 3
$V_{environmental}$	First order stream. Default volume of 1 500 m <sup>3</sup> or disposal outfall flow	Bioregional definitions for flow conditions observed selected streams	Accounts for variability of the bioregional stream
$V_{contaminated}$	Volumes as defined by release scenario. Further refinement is not required	Volumes as defined by release scenario. Further refinement is not required	Volumes as defined by release scenario. Further refinement is not required
$V_{uncontaminated}$	Default volume of 0 m <sup>3</sup>	Potential for uncontaminated water sources considered	Potential for uncontaminated water sources considered

Contaminated water may include flowback and produced water that is released from a storage dam during an overflow event. Uncontaminated water may include runoff waters from an uncontaminated part of the catchment.

The selection of  $V_{environmental}$  will be conducted on a tiered basis. Initially, a hypothetical natural aquatic ecosystem representative of a low flow stream or shallow small wetland area able to sustain aquatic life will be considered (Tier 1). The US EPA (2001) found that using this methodology it was able to predict, reasonably well, upper level contaminant concentrations of chemicals used in agriculture in small but ecologically important upland streams. For the assessment being undertaken here, the aquatic ecosystem is assumed to be situated in the vicinity of coal seam gas extraction operations, such that operations in the catchment area will directly impact the aquatic ecosystem. The assumed volume of the aquatic ecosystem will be large enough not to be ephemeral (existing only for a short time) and that contamination from coal seam gas extraction activities will generally result in dilution

of the chemical in the contaminated water. To provide upper bound estimates, the volume of contaminated water will be assumed to be much greater than the environmental water volume ( $V_{\text{contaminated}} \gg V_{\text{environmental}}$ ). However, scenarios such as spills of neat chemical (i.e. at 100% concentration) and slow leaks from dams (containing flowback or produced water) are likely to be exceptions rather than the norm. Other potential exceptions to this include the discharge of wastewater for supplementation of environmental flows, or use in aquaculture with subsequent disposal of water to surface water bodies (as described in Section 2.2.4). In the absence of natural base flows, the discharged water may in itself become a habitat for aquatic life, particularly during extended dry periods.

The selection of  $V_{\text{environmental}}$  in higher tiers of assessment will be based on the volume of permanent watercourses within the six priority areas [as described in DoEE (2017a)], which are proximal to coal seam gas extraction activities and have actual measured environmental flow volumes. It is expected that such watercourses will be 4<sup>th</sup> order or higher streams. Where appropriate, watercourses with the most potential to support Matters of National Environmental Significance [MNES, as defined under the *Environment Protection and Biodiversity Conservation Act 1999* (EPBC Act)], such as Ramsar sites, will be given precedence for assessment. Such watercourses would necessarily be downstream of existing or anticipated coal seam gas activity and in the same catchment.

#### 3.3.1.1. Volume of environmental water

The environmental volume will be selected as a surrogate for multiple exposure route effects in Tier 1 to represent the bounding estimate. The environmental volume ( $V_{\text{environmental}}$ ) is described in Section 3.3.1. For natural flow, a default daily flow of a low flow first order stream may be used in Tier 1 (corresponding to approximately 0.03 to 0.06 m/sec, or 0.1 to 0.2 km/hr), where the primary stream is approximately 2 m wide and 25 cm deep (based on Steels, Pauls and Dixons Creek Environmental Flows Technical Panel [SPDEFTP (2003)]). This volume is also representative of a pond 15 cm deep, with a surface area of 1 ha. This scenario is considered most appropriate for exposure from accidental releases to an existing natural aquatic ecosystem. The low flow of the aquatic ecosystem will be reflected by the small catchment area for that aquatic ecosystem, such that only a few coal seam gas operations would occur in that area. It is highly unlikely that multiple accidental releases would occur simultaneously to the aquatic ecosystem.

However, discharged water may in itself become the habitat for aquatic life where there is little or no natural base flow during extended dry periods. In this case, the flow of the environmental aquatic ecosystem is assumed to equal the outfall of the disposal of wastewater. This may also act as a surrogate for multiple releases over an area, as the bounding estimate concentrations of contaminants at outfall cannot be exceeded regardless of how many coal seam gas operations are releasing in an area (due to the dilution factor introduced by the multiple releases).

For a Tier 2 assessment the volume will be selected from a conservative single-point value derived from low flow conditions observed in the model river(s) [after US EPA (1992)]. It is expected that the identified model rivers will have an approximate stream order of 4 or higher. In a Tier 3 assessment, the typical variability of volume for the model river(s) will be considered. Values for flow such as 10<sup>th</sup> or 25<sup>th</sup> percentile of the flow duration curve will be considered.

#### 3.3.1.2. Volume of contaminated water

The contaminated volume  $V_{\text{contaminated}}$ , will generally simply be the volume of water in which the contaminant is released. This would be the volume of the spill or overflow in cases of an accidental release. For intentional releases, the volume will simply be the volume discharged depending on the release scenario. If the release is continuous then volume should be

considered for a fixed timeframe (e.g. one day), which is the same as that of the timeframe considered for the flow rate of the receiving environment (e.g. 1500 m<sup>3</sup> per day). For runoff, the volume of contaminated water may be determined from the area over which the contaminant is spread in hectares<sup>2</sup>. Where this area is not defined (due to the use of wastewater as dust suppression and irrigation), the volume may be calculated on a per hectare basis. This has the advantage that provided the rate of application of contaminant per hectare is known, “an edge of field” concentration may be calculated independent of the size of the field, as the concentration is equal to the quantity per hectare, divided by the volume runoff per hectare, such that the area values effectively ‘cancel out’.

In Tier 1 the runoff in mm from a soil type, which results in the highest concentration of contaminant will be used. In Tier 2, a regional value for runoff based on regional soil type will be used. In Tier 3, the probability of rainfall resulting in runoff, which contains concentrations of chemicals exceeding a level of concern, will be introduced.

### 3.3.1.3. Volume of uncontaminated water

The uncontaminated volume ( $V_{uncontaminated}$ ), in cases like spills or intentional releases directly to a watercourse, will be zero. This will be regarded as the default value for Tier 1 regardless of the scenario. The uncontaminated volume is most relevant to runoff scenarios where the runoff may come from contaminated and uncontaminated areas.

For runoff, the volume may be calculated in the same manner as for  $V_{contaminated}$ , except that the area is uncontaminated. For a given catchment for an aquatic ecosystem, this area will be equal to the catchment area less the contaminated area. Initially, a hypothetical catchment may be used where only under limited soil and meteorological conditions would it be able to sustain the environmental water body being considered. This would result in a smaller volume of  $V_{uncontaminated}$ , than more realistic scenarios and hence the concentration would be higher. For an initial consideration for Tier 1, the catchment size may be considered to be 10 ha, supporting a 1 500 m<sup>3</sup> aquatic ecosystem. In higher tiers, more realistic catchments for 4<sup>th</sup> order or higher streams may be used. However, double counting of  $V_{uncontaminated}$  must be avoided, as the measured flow rate may already have taken into account runoff from uncontaminated areas.

The area over which the contaminated water is spread and depth to which it penetrates may be regarded as the soil receiving environment. The PEC in the terrestrial compartment ( $PEC_{soil}$ ) from a single release event may therefore similarly consider simple dilution of the chemical in soil using Exposure Equation 4:

$$PEC_{soil} = \frac{Q}{A \times d \times \rho} \times 10^6 \text{ mg/kg} \quad [\text{Exposure Equation 4}]$$

Where:

$PEC_{soil}$  = Predicted environmental concentration in the soil compartment

Q = Chemical quantity (kg)

A = Area over which contaminant is spread (m<sup>2</sup>)

d = Depth to which the contaminant penetrates (m)

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<sup>2</sup> Multiplying the amount of runoff water (in mm) by 10 000 (m<sup>2</sup>/ha) and dividing by 1 000 (mm/m) converts the units to m<sup>3</sup>. The runoff in mm is calculated from Exposure equation 9 (Section 3.4.2), with the use of an appropriate conversion factor from inches to mm (× 25.4 mm/inch).

$\rho$  = Density of the soil (kg/m<sup>3</sup>)

#### 3.3.1.4. Area

Operational needs of irrigation or dust suppression will determine the area over which flowback and produced water (whether treated or untreated) is used (DoEE 2017a). Standard assumptions for the area to consider for the exposure scenarios where there is intentional application of wastewater that may contain chemicals to the soil compartment are derived in Section 4.3.2.

For spills, the area and depth of penetration will be dependent on the rate of spill, soil properties, and physical properties of the liquid spilled. A simple estimate of spill height, which may be used to calculate spill area is reported by Keller and Simmons (2005) and is presented in Exposure Equation 5:

$$h = \sqrt{\frac{1 - \cos(\beta) \times \sigma}{\rho \times g}} \quad [\text{Exposure Equation 5}]$$

Where:

$h$  = Spill height (or head above surface normal to surface) (cm)

$\beta$  = Contact angle specific to the soil surface tension

$\sigma$  = Soil surface tension in poise

$\rho$  = Liquid density (g/cm<sup>3</sup>)

$g$  = Gravitational acceleration (cm/sec<sup>2</sup>)

The area may then be simply calculated for Exposure Equation 6 as follows:

$$A = \frac{V}{h} \quad [\text{Exposure Equation 6}]$$

Where:

$A$  = Area

$V$  = Volume of the spill

$h$  = Spill height

If a spill occurs and the area over which it is predicted to spread out exceeds the amount of land in that area, then contamination by flow overland of chemicals to nearby waterways may occur.

#### 3.3.1.5. Depth

The depth to which the contaminant initially penetrates will vary depending on the condition of the soil to which it is applied. In the bounding estimate (Tier 1), the minimum depth to which the contaminant is likely to penetrate will be considered. A refinement of this scenario (Tier 2) will consider more likely depths based on industry practices and regional information. In both of these tiers, the depth to which the contaminant penetrates is considered to be fixed.

However, over time the contaminant is expected to leach from the soil mixing zone to lower depths where the contaminant will not be available to plants or for runoff. The

US EPA (2005a and 2005b) has recommended calculations, Exposure Equation 7, for leaching which are dependent on the physico-chemical properties of the contaminant, which may be considered in Tier 3 assessment. Moreover, the groundwater conceptualisation by Mallants et al. (2017c) derives dilution factors (using a tiered approach) to estimate the concentrations of chemicals leached over time to groundwater ecosystems. This information may be used at higher tiered levels of assessment for undertaking mass balance<sup>3</sup> calculations to determine accurate chemical concentrations moving into the different environmental compartments.

### 3.3.1.6. Density

The density of soil will vary depending on locality. However, default values based on averages of measured values will be used. These are discussed in Section 4.3.2.

### 3.3.1.7. Repeated applications

Where repeated applications of contaminants are likely to occur as a result of irrigation or dust suppression on roads, the accumulation will be modelled according to Equation 8, Equation 9, Equation 10, and Equation 11. However, for contaminants which do not degrade rapidly (including many geogenic chemicals) the value of  $PEC/PEC_0$ , will simply approach infinity with repeated applications, assuming no losses. Therefore, losses from the mixing zone of the soil via leaching and runoff would need to be incorporated into the analysis. Exposure Equation 7 was developed by the US EPA (2005a; 2005b) to describe losses of contaminant from the mixing layers of soil. The value for  $k_{yr}$  may then be used in Equation 7 as the value for  $k_r$  to calculate the steady state PEC. The steady-state PEC will still be limited by the physical properties of the contaminant and this limitation may be considered to be the limit of water solubility (Mallants et al. 2017b).

$$k_{yr} = \frac{\Psi_{yr} + \Psi_{irr} - E_v - R_{yr}}{\theta_{sw} \times d \times [1 + (Kd \times \rho \div \theta_{sw})]} \quad [\text{Exposure Equation 7}]$$

Where:

$k_{yr}$  = Loss constant of contaminant due to leaching ( $\text{yr}^{-1}$ )

$\Psi_{yr}$  = Average annual precipitation (cm/yr)

$\Psi_{irr}$  = Average annual irrigation (cm/yr)

$E_v$  = Average annual evapotranspiration (cm/yr)

$R_{yr}$  = Annual runoff (cm/yr)

$\theta_{sw}$  = Soil volumetric water content ( $\text{mL water/cm}^3$  soil), default =  $0.2 \text{ mL/cm}^3$

$d$  = Soil mixing zone depth (cm)

$Kd$  = Soil/water partition coefficient ( $\text{mL water/g soil}$ )

$\rho$  = Soil bulk density ( $\text{g soil/cm}^3$  soil)

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<sup>3</sup> However, mass balance calculations can only be undertaken if there is enough information to match the two sets of estimated concentrations (for surface and subsurface environments) at each tier.



The losses of chemical from the mixing zone due to leaching will potentially enter the underlying shallow aquifers. The modelling of contamination of shallow groundwater systems is addressed in a separate companion report (Mallants et al. 2017b).

Exposure Equation 7 will be further evaluated for its appropriateness and data availability during the risk assessment.

### 3.3.2. Air PECs

Toxic effects from exposure of organisms to airborne contaminants in the environment are rarely studied. Hence, even if a PEC for the atmosphere is calculated it can only rarely be used to infer environmental effects (EPHC 2009a) given the lack of environmental exposure guidelines. In addition, the atmospheric environmental compartment is highly dynamic, with changes in wind velocity, direction, temperature, and humidity. Without knowledge of these parameters (and others), the uncertainty in the PEC is likely to be large. Due to limited use and difficulty in estimating the PEC, qualitative screening assessments are generally conducted in Australia for the atmospheric exposure pathway (EPHC 2009a and 2009b). However, an approximation of the PEC in air may be calculated as described generally in Exposure Equation 8:

$$PEC_{air} = E_{local} \times K_{air} \quad \text{[Exposure Equation 8]}$$

Where:

$PEC_{air}$  = Local concentration in air during emission episode in  $\text{mg/m}^3$

$E_{local}$  = Local direct emission rate to air in  $\text{kg/day}$

$K_{air}$  = Concentration in air at source strength of  $1 \text{ kg/d} = 2.78\text{E-}04 \text{ mg/m}^3$

The value for  $K_{air}$  is based on the assumption that the source is 100 m away (based on the distance to the boundary fence for many industrial operations), the emission source is 10 m above ground, and that there is limited transformation of the chemical from reactions in the atmosphere. This model was developed to estimate concentrations where daily emission data from coal seam gas sites is available from a point source. This was not designed to estimate concentrations in air originating from chemicals in coal seam gas storage ponds. However, a bounding estimate may be made for chemicals in storage ponds based on the assumption that volatile chemicals will rapidly reach equilibrium partitioning between air and water in accordance with Henry's Law. Therefore if the quantity of chemical in a volume of liquid is known, then the emissions in one day may be considered to be the amount of partitioning from the water.

## 3.4. Chemical fate in the environment

### 3.4.1. Preliminary comments on intentional releases

The release of contaminants may be accidental or intentional. Intentional releases are usually associated with the use and disposal of backflow or produced water under managed and regulated conditions. Current management options for this water include surface discharge, underground injection, impoundment with no re-use (evaporation or recharge) and beneficial uses including aquaculture, coal washing, industrial operations, irrigation, and watering of feedlots. The preferred management method is dependent on volume of water, salinity levels and chemical composition, as well as local climate, surface drainage and environmental regulations. This has led to site-specific solutions, which are also liable to change as legislative requirements and / or industry practices change. As methods for management of backflow and produced water may change over time, it is not feasible to

specify a precise pattern of disposal. Instead, the likely fate of the contaminants for each potential disposal method is considered. This has the advantage of identifying which disposal method is likely to have the smallest environmental impact.

### 3.4.2. Runoff

Several exposure scenarios will result in either the accidental or intentional exposure of soil to contaminants. This contamination has the potential to enter the aquatic environment when a rainfall event results in runoff, transporting the soil-bound contaminant to a nearby aquatic ecosystem or watercourse.

The approach in Exposure Equation 9 [Australian Pesticides and Veterinary Medicines Authority (APVMA) 2010; based on Probst et al. (2005)] recognises that runoff is just one component of a wider issue of mass balance of chemicals in the environment. It was chosen on the basis that it has relatively few inputs but still considers what many authors and regulatory agencies consider the most important factors in determining the runoff of chemicals [Department of Sustainability, Environment, Water Population and Communities (DSEWPoC) 2009]. These factors include the amount of precipitation and runoff; the topography of the land, particularly slope; soil and vegetation characteristics; and physico-chemical characteristics of the contaminant.

$$L\%_{\text{runoff}} = \left(\frac{R}{\Psi}\right) \times Cr_{\text{soil\_surface}} \times f1_{\text{slope}} \times f2_{\text{bufferzone}} \times f3_{\text{foliar\_application}} \times \text{heterogeneity\_factor} \times 100 + \text{suspended\_contaminants}\% \quad [\text{Exposure Equation 9}]$$

Where:

$L\%_{\text{run-off}}$  = Percentage of released chemical

$R$  = Runoff (mm/day)

$\Psi$  = Precipitation (mm/day)

$Cr_{\text{soil\_surface}}$  = Variable dependent on degradation kinetics of the contaminant and soil adsorption (see Section 4.4.1 for default values for Exposure Equation 10)

$f1_{\text{slope}}$  = Variable dependent on slope (see Exposure Equation 11)

$f2_{\text{bufferzone}}$  = Variable dependent on filtering (see Exposure Equation 12) (buffer default = 1 [no effect])

$f3_{\text{foliar\_application}}$  = Parameter dependent on interception and retention by foliage (see Exposure Equation 13)

$\text{heterogeneity\_factor}$  = Parameter which allows for partial area runoff, set between > 0 and < 1

$\text{suspended\_contaminant}$  = Contaminant adsorbed to particulates and held in suspension

$$Cr_{\text{soil\_surface}} = e^{(-3 \ln 2 \div DT50_{\text{soil}})} \times [1 \div (1 + Kd)] \quad [\text{Exposure Equation 10}]$$

Where:

$Kd$  = The water soil partitioning coefficient (L/kg)

$DT50$  = This half-life of a substance in soil (days)



See Section 4.4.1 for default values.

$$f1_{slope} = 0.02153 \times slope + 0.001423 \times slope^2 \text{ for } slope < 20\% \\ = 1 \text{ for } slope \geq 20\% \quad [\text{Exposure Equation 11}]$$

Where:

Slope = Slope in % (i.e., rise over run – to convert degrees to percent slope use  $\tan \Theta \times 100$ )

DT50 = half-life of a substance in soil (days)

$$f2_{bufferzone} = 0.83^{buffer\ width} \quad [\text{Exposure Equation 12}]$$

Where:

buffer width = Width of buffer zone able to filter chemicals from runoff water (m)

$$f3_{foliar\_application} = 1 - F_{int} \times 0.5 \quad [\text{Exposure Equation 13}]$$

Where:

$F_{int}$  = The fraction of chemical intercepted by foliage when applied by spray or overhead irrigation (unitless)

For the bounding estimate Tier 1 scenario contaminants are assumed to be dissolved in water, have no affinity for soil ( $Kd = 0$ ) and do not degrade ( $DT50 = \infty$ ), such that  $C_{r_{soil\_surface}} = 1$ . Slopes are also considered to be the steepest for a particular use since this will maximise the potential for runoff and transport to a receptor. Buffer zones are considered not to be in place or if they are, to have no effect. Also, all of the contaminated area is considered to contribute equally to runoff. The amount of suspended chemical is initially regarded as 0, assuming that all of the chemical is present in its most mobile and available form.

During rainfall, a portion of the water will infiltrate into the soil to be taken up by plants, evaporate or penetrate deeper into shallow groundwater, while the remainder will run off and enter the aquatic compartment. Similarly, contaminants on the soil surface, which become dissolved in this water will either infiltrate into soil or run off. The quantity of the contaminant in runoff water is proportional to the ratio of the amount of runoff and the total water input, that is, the precipitation ( $L\%_{run-off} \propto R/\Psi$ ). The amount of rainfall may be based on regional rainfall data and use the highest rainfall values to represent the bounding estimate in Tier 1 (more representative values are used in Tier 2). A standard methodology to calculate this relationship has been developed by the NRCS (1986) as shown in Exposure Equation 14:

$$R = (\Psi - 0.2S)^2 / (\Psi + 0.8S) \quad [\text{Exposure Equation 14}]$$

Where:

R = Runoff (inches<sup>4</sup>)

Ψ = Precipitation (inches)

S = Potential maximum retention after runoff begins in inches, calculated from  
 $S = 1\,000 / CN - 10$  (where CN is an empirical value, namely the curve number for soil), as described in NRCS (1986)

The amount of runoff water from soil is dependent on the amount of rainfall and the condition of the soil, which may be affected by parameters such as moisture content, land use and ground cover.

Merz (2008) describes how Exposure Equation 14 has been developed through the work of Lutz (1984) and Maniak (1988) to better account for soil moisture and soil texture (see 0 for further details). Their findings for some soils have been published in tabulated form by the OECD (2000) and were recently used by DSEWPaC (2012) to assess the potential of runoff for diuron. During this risk assessment, the runoff versus rainfall data for the soils published by OECD (2000) was reviewed to determine its applicability to soils exposed to contaminants from coal seam gas extraction activities.

To determine a bounding estimate scenario for precipitation and runoff, two competing considerations will need to be taken into account. As runoff increases, the percentage of contaminant mobilised will increase. However, the volume of runoff water will also increase, thereby potentially decreasing the concentration of the contaminant in the runoff water. These considerations will need to be optimised for various soil types to find the precipitation scenario resulting in the highest concentration in the runoff water.

In a Tier 2 assessment consideration will be given to chemical properties, which affect soil affinity and degradation. Where values for soil affinity ( $K_d$ ) are not available an estimate may be made from the soil organic carbon-water partition coefficient ( $K_{oc}$ ), provided that the major route of binding to soil is through the organic carbon (OC) content. Exposure Equation 15 describes how affinity for soil of a contaminant is related to affinity to organic carbon:

$$K_d = K_{oc} \times OC\% \div 100 \quad [\text{Exposure Equation 15}]$$

Where:

$K_d$  = The water soil partitioning coefficient (L/kg)

$K_{oc}$  = The water organic carbon partitioning coefficient (L/kg)

$OC\%$  = The weight percentage of organic carbon in soil (unitless)

In addition, more realistic values for slope, influence of foliar application and areas that do not contribute effectively to runoff (heterogeneity\_factor < 1) may be considered. The effectiveness of buffer zones are not well understood and are not included. However, sediment transport is considered for chemicals that bind strongly to soil. With some exceptions these chemicals will generally have water solubility of less than 1 mg/L.

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<sup>4</sup> An inch is defined as 25.4 mm exactly <[http://www.npl.co.uk/reference/faqs/on-what-basis-is-one-inch-exactly-equal-to-25.4-mm-has-the-imperial-inch-been-adjusted-to-give-this-exact-fit-and-if-so-when-\(faq-length\)>](http://www.npl.co.uk/reference/faqs/on-what-basis-is-one-inch-exactly-equal-to-25.4-mm-has-the-imperial-inch-been-adjusted-to-give-this-exact-fit-and-if-so-when-(faq-length)>), accessed 18 July 2013.

To calculate the percentage of suspended contaminant it is possible to use empirical data on erosion of soil per unit area under various rainfall conditions and compare with the amount of contaminated soil, using Exposure Equation 16:

$$\text{suspended\_contaminant}_{\%} = \frac{M_{\text{eroded\_soil}}}{M_{\text{contaminated\_soil}}} \times 100$$

[Exposure Equation 16]

Where:

$M_{\text{eroded\_soil}}$  = Quantity of soil eroded in a unit area (kg/ha)

$M_{\text{contaminated\_soil}}$  = Quantity of soil contaminated in a unit area (kg/ha)

The amount of contaminated soil ( $M_{\text{contaminated\_soil}}$ ) is calculated from Exposure Equation 4.

Not all rainfall events will result in runoff and even if runoff does occur, the concentration of contaminants in that runoff water may be below levels of environmental concern. It is expected that climatic conditions will determine the likelihood of rainfall and runoff containing contaminants above a level of environmental concern. For the Tier 3 assessment, this probability of runoff resulting in concentrations of contaminants above a level of concern will be determined. This determination may be made by considering the probability on any one day of rainfall exceeding a particular value where this would cause contamination levels of concern. The probability considers the chance of rainfall on any particular day and the cumulative probability of the rainfall. For example, in Hay, New South Wales, 93% of all rainfall events are 12 mm/day or less, and thus only 7% of rainfall events exceed 12 mm/day. However, rainfall does not occur every day in Hay. As the chance of rainfall occurring and the chance of it exceeding a certain value are independent events, the probability of rainfall exceeding a certain value on any one day is equal to the probability of rainfall occurring multiplied by the probability that, when rainfall occurs, it will exceed a certain value.

#### 3.4.2.1. Model limitations

The runoff model is necessarily simplified, but it attempts to account for the major influences on contamination of environmental waters by runoff. Several assumptions have been made in developing the model and many of these are not entirely realistic. However, the approach is conservative, such that the concentrations predicted are likely to be above the actual concentrations and other influences are expected to be small in comparison to the parameters used in the model.

Particular areas that have been deliberately simplified are as follows:

- Groundwater quality can influence the quality of surface water. Modelling of contamination of surface water by groundwater is further advanced by Mallants et al. (2017b). It is assumed here that contaminated groundwater has less influence on peak concentrations of contaminants than direct runoff from contaminated soil for short-term exposure, although this is likely to be site- and chemical-specific.
- The actual amount of contaminant that runs off foliage will be dependent on many factors. These will include the fate of the chemical on the leaves (including half-life and volatilisation), formulation, the type of foliage and the intensity of the rain. This is only partially addressed by the model. A simplistic approach is taken where it is assumed that half of the contaminant that is intercepted is retained on the foliage. This is justified by the findings of Linders et al. (2000), citing Willis et al. (1994). However, this should be treated with caution as only two contaminants under one set of conditions were tested.

- The model assumes that the partitioning of the contaminant between the soil and aqueous phases has attained equilibrium. In reality, runoff may occur before equilibrium between the two phases is reached.
- The actual proportion of contaminant transported by sediment will be a function of the amount of sediment eroded and the  $K_d$  value of the contaminant. The model simply uses the water solubility of the contaminant as the determinant for validity of the aqueous transport component of the model. However,  $K_d$  and water solubility correlate well in many cases and the maximum likely amount of sediment erosion can be taken into account. Field studies supported the view that the 1 mg/L water solubility cut-off was reasonable (Kookana 1998; CSIRO undated).

### 3.4.3. Dust transport

In addition to runoff, contaminants may be attached to dust and become airborne. This dust may then come into contact with other environments, including water bodies. The percentage of contaminants transported to surface water bodies in this manner is expected to be small compared to the amount transported by other mechanisms such as runoff. However, this should be confirmed by reviewing site monitoring data. To calculate the percentage of airborne dust contaminants, empirical data on wind erosion of soil per unit area may be used under various wind and soil conditions and compared with the amount of contaminated soil as described generally by Exposure Equation 17:

$$\text{airborne\_dust\_contaminant}_{\%} = \frac{M_{\text{airborne\_eroded\_soil}}}{M_{\text{contaminated\_soil}}} \times 100$$

[Exposure Equation 17]

Where:

$M_{\text{airborne\_eroded\_soil}}$  = Quantity of soil eroded in a unit area (kg/ha)

$M_{\text{contaminated\_soil}}$  = Quantity of soil contaminated in a unit area (kg/ha)

The amount of contaminated soil ( $M_{\text{contaminated\_soil}}$ ) is calculated from Exposure Equation 4.

Where empirical data for the quantity of soil that becomes airborne is not available, it may be estimated using the equation developed by Cook and Doornkamp (1973), which is described in Exposure Equation 18:

$$q_{\text{soil}} = a \times (D_e)^{\frac{1}{2}} \times \frac{\rho}{g} \times (V_*)^3$$

[Exposure Equation 18]

Where:

$q_{\text{soil}}$  = Quantity of soil in mass/area/time (e.g. g/cm<sup>2</sup>/sec)

$a$  = Coefficient dependent on size distribution of erodible particles (unitless)

$D_e$  = Average equivalent diameter of soil particles (cm)

$\rho$  = Density of air (g/cm<sup>3</sup>)

$g$  = Acceleration due to gravity (cm/sec<sup>2</sup>)

$V_*$  = Drag velocity above the eroding surface (cm/sec)

This Exposure Equation was further evaluated for its appropriateness to the National Coal Seam Gas Chemicals Assessment, including data availability, during the risk assessment.

### 3.4.4. Volatilisation from water

Chemicals in water including dams, streams and lakes may volatilise and enter the atmosphere. The relative concentrations in each compartment ( $K_{\text{air-water}}$ ) for a closed system (no exchange of air or water) at equilibrium at a given temperature may be calculated in the air based on the Henry's Law Constant as described in Exposure Equation 19:

$$K_{\text{air-water}} = H/RT \quad [\text{Exposure Equation 19}]$$

Where:

$K_{\text{air-water}}$  = Air-water partition coefficient (unitless)

$H$  = Henry's Law Constant ( $\text{Pa m}^3/\text{mol}$ )

$R$  = Gas constant ( $\text{J/K mol}$ )

$T$  = Absolute temperature in Kelvin (K)

Once the equilibrium constant has been established it may be used to calculate the concentration in air with respect to the concentration in the aquatic ecosystem according to Exposure Equation 20:

$$PEC_{\text{air}} = K_{\text{air-water}} \times PEC_{\text{water}} \quad [\text{Exposure Equation 20}]$$

Where:

$PEC_{\text{air}}$  = Concentration of chemical volatilised from the water column ( $\text{mg/L}$ )

$K_{\text{air-water}}$  = Air-water partition coefficient (unitless)

$PEC_{\text{water}}$  = Predicted environmental concentration in the aquatic ecosystem and / or watercourse ( $\text{mg/L}$ )

### 3.4.5. Partitioning and sedimentation

#### 3.4.5.1. Partitioning

Aquatic systems are also comprised of sediment at the bottom and particulate matter suspended in the water column. Chemicals in water bodies may adsorb to this sediment and other particulate matter, depending on their affinity for particulates. The chemical's affinity for the sediment and particulates may change in response to changes in pH or temperature, but studies are usually conducted under conditions representative of the natural environment. Generally, the amount of sediment at the bottom of the aquatic system will greatly outweigh the amount of suspended particulates in the water column and partitioning to the sediment at the bottom of the aquatic system will be the predominant mechanism of chemical movement.

In this case, the PEC in sediment can be calculated using the following methodology (EPHC 2009b). The solid-water partition coefficient in sediment ( $K_d$ ) can be calculated based on a chemical's affinity for sediment using Exposure equation 15. However, the equilibrium partitioning behaviour of a chemical is dependent on the ratio of water and sediment in a system. The coefficient is a normalised value, where the ratio of water to sediment is 1 L to 1 kg. To account for the makeup of the aquatic system the ratio of water to sediment in L to kg must be calculated. This may be done assuming 80% water and 20% solids (by volume)

and converting the amount of solids to mass by multiplying by the density as described in Exposure Equation 21:

$$K_{\text{sediment\_water}} = 0.8 + (0.2 \times K_d / 1000) \times \rho_{\text{solid}}$$

[Exposure Equation 21]

Where:

$K_{\text{sediment\_water}}$  = Solid-water partition coefficient in sediment (L/kg)

$K_d$  = The water soil partitioning coefficient (L/kg)

$\rho_{\text{solid}}$  = Bulk density of solid phase only (Kg/m<sup>3</sup>)

This will determine the partitioning of chemicals to the sediment. The concentration in sediment may then be calculated from the concentration of the chemical in water multiplied by the partitioning coefficient to sediment. To convert this value to mg/kg sediment it must be divided by the density of the sediment (and multiplied by 1 000 to convert to mg/kg). This is represented by Exposure Equation 22:

$$PEC_{\text{sediment}} = K_{\text{sediment\_water}} / \rho_{\text{sediment}} \times 1000 \times PEC_{\text{water}}$$

[Exposure Equation 22]

Where:

$PEC_{\text{sediment}}$  = Predicted environmental concentration in sediment (L/kg)

$\rho_{\text{sediment}}$  = Bulk density of sediment including pore water (Kg/m<sup>3</sup>)

$PEC_{\text{water}}$  = Predicted environmental concentration in water (mg/L)

### 3.4.5.2. Sedimentation

As previously mentioned, sedimentation firstly involves the adsorption of chemicals to suspended particles. These particles may then settle to the sediment layer. Highly adsorptive substances are often not in equilibrium distribution between water and solids due to their cohesion to the suspended matter (EPHC 2009b). Similarly, where suspended matter in the water column is significant, sedimentation will need to be considered. This is most likely to occur where flowback and produced water or drilling fluids contain significant quantities of suspended matter. In this case, the amount of sediment coming out of suspension would be affected by many factors including the size of particulates, ability of particulates to aggregate, currents in the water and temperature of the water.

### 3.4.6. Degradation in the environment

Many chemicals degrade or are attenuated in the environment by biotic (biological) and / or abiotic (physical and chemical) processes. For industrial chemicals, an assessment of the potential of the chemical to biodegrade in the environment is made by studying the biodegradation of the chemical in the soil sample using tests such as OPPTS 835.3180 described by the US EPA Guideline for the Testing of Chemicals<sup>5</sup>. Hydrolysis is often a major mode of abiotic degradation and the potential for industrial chemicals to hydrolyse in the

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<sup>5</sup> Fate, Transport and Transformation Test Guideline OPPTS 835.3180 Sediment/Water Microcosm Biodegradation Test: [http://www.d.umn.edu/~pschoff/documents/EPA-OPPTS\\_Sed-WaterBioD.pdf](http://www.d.umn.edu/~pschoff/documents/EPA-OPPTS_Sed-WaterBioD.pdf)

environmental pH range (4 to 9) is routinely measured (EPHC 2009a). Other studies conducted on the fate of chemicals in the environment include aqueous photolysis, soil photolysis, aerobic and anaerobic soil degradation, aerobic and anaerobic degradation in water / sediment systems (EPHC 2009b). Where only the ready biodegradation test rate is available for a chemical, this may be extrapolated to other environmental compartments according to the following conversions (EPHC 2009a, citing (EC) 2003).

Table 3.3 First order rate constants and half-lives for biodegradation in surface water estimated based on results of screening tests on biodegradability

Study result	Rate constant ( $k_{\text{biowater}}$ , $\text{d}^{-1}$ )	Water half-life (d)
Ready biodegradable	0.047	15
Ready, but failing the 10-d window	0.014	50
Inherently biodegradable	0.0047	150
Not biodegradable	$6.93 \times 10^{-7}$	~1 000 000

Table 3.4 First order rate constants and half-lives for biodegradation in surface water estimated based on results of ready and inherent biodegradability test results

Ready test result (% biodegradation)	Inherent test result	Rate constant ( $k_{\text{biowater}}$ , $\text{d}^{-1}$ )	Water half-life (d)
pass test	-	0.1400	5
fail test, but $\geq 40\%$	-	0.0690	10
fail test, $\geq 20\%$ , but $< 40\%$	$\geq 70\%$	0.0230	30
-	$\geq 20\%$ , but $< 70\%$	0.0069	100
fail test, $< 20\%$	$< 20\%$	0.0000	$\geq 10\,000$

Table 3.5 Half-lives for biodegradation in surface soil in days estimated based on results of screening tests on biodegradability and based on water-solid partition coefficient  $K_d$

$K_d$ (L/kg)	Soil half-life (d)		
	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
$\leq 100$	30	90	300
$>100, \leq 1\,000$	300	900	3\,000
$>1\,000, \leq 10\,000$	3\,000	9\,000	30\,000

Where the ready biodegradation rate is not available, a quantitative structure activity relationship (QSAR) model [Laboratory of Mathematical Chemistry (LMC) 2011] may be used to infer the rate for a chemical, provided that an appropriate QSAR model is available for that class of chemical.

In all cases, first order (or pseudo first order) kinetics will be assumed unless there is clear evidence that demonstrates that other kinetic approaches are appropriate. Inorganic compounds and trace elements are unsuited to this degradation analysis.

### 3.5. Quantity of chemical released

During coal seam gas extraction activities there could potentially be several points of release. The PEC calculations require an estimate of the potential quantity (Q) released from each of the lifecycle stages and are based on the approach described by Rozell and Reaven (2012), unless otherwise stated. The assumptions and calculations that may apply at each assessment tier are also described. In Tier 3, the probability of a release from incidents such as spills and overflows is considered. In general, if sufficient data are available a histogram of release size versus release frequency may be constructed. These data may be extrapolated using a Monte-Carlo type analysis to analyse the probability of the events occurring (US EPA 2004).

#### 3.5.1. Transport exposure equations

Coal seam gas extraction activities require transportation of a significant amount of chemicals to intermediate storage sites and from there to well sites (NICNAS 2017a and 2017b; DoEE 2017a). Environmental exposure may occur as a result of truck accidents. Release Equation 1 can be used to estimate the quantity of the spill ( $Q_{xT}$ ):

$$Q_{xT} = Q_T \times i_T \quad \text{[Release Equation 1]}$$

Where:

$Q_{xT}$  = Quantity released from transport accidents

$Q_T$  = Quantity of drilling or hydraulic fracturing chemical transported

$i_T$  = Portion of a truck load that would spill in a crash

Rather than relying on there being sufficient data to construct a histogram of the frequency of releases of different sizes, the probability of transport accidents has been extrapolated from data on transport accidents in general. The probability ( $P_T$ ), excluding the chance of a truck accident occurring twice for the same truck, is described in Release Equation 2:

$$P_T = 2 \times \frac{N_C}{N_S} \times i_{TC} \quad \text{[Release Equation 2]}$$

Where:

$P_T$  = Probability of transport accident involving drilling or hydraulic fracturing chemicals

$N_C$  = Number of truck crashes per year

$N_S$  = Total number of shipments per year

$i_{TC}$  = Portion of trucks that crash resulting in a spill

Using a tiered approach and starting at Tier 1, the initial bounding estimate scenario considered that the entire contents of a truck ( $Q_T$ ) are spilled. In this case  $Q_T$  will be assumed to be the maximum amounts likely to be transported and the full truck load spilled (i.e.  $i_T = 1$ ). The methodology for deriving  $Q_T$  values for transport to intermediate and individual wells sites is outlined in Section 4.2.1.

However, not all accidents will involve trucks carrying their full capacity. Rather, it is more likely that volumes transported will reflect industry practice including packaging sizes for chemicals. Accordingly in Tier 2, more realistic volumes for  $Q_T$  will be considered. In addition,



values of  $i_T$  of less than 1 may be considered if there is sufficient evidence to demonstrate that the entire contents are unlikely to spill in an accident.

For the purposes of this assessment, it is assumed from information obtained in the literature review (DoEE 2017a) that two journeys are made for each fracturing operation (one to the site and one return), acknowledging that more journeys may be required. In a bounding estimate case, it will be assumed that the entire quantity of chemicals is returned due to postponement or cancellation of fracturing or drilling operations. The risk may be considered in the conventional manner of determining the magnitude of the effect and the probability of that effect occurring.

A limitation of this method is that the probability of truck accidents will be based on generic, historic data. It does not take into account specific coal seam gas industry practices or future trends, such as increased road traffic due to an increase in coal seam gas extraction activities in an area.

### 3.5.2. Storage exposure equations

Chemicals used for hydraulic fracturing and drilling are usually transported first in bulk to a regional holding facility before smaller amounts are delivered as required to operational well sites. It is assumed that such regional warehouses serve several well sites. Exposure at the central storage facility may occur through leaking containers or accidental breakage and mishandling of fluids during blending. Release Equation 3 will be used to assess this aspect:

$$Q_{xS} = Q_S \times i_S \quad \text{[Release Equation 3]}$$

Where:

$Q_{xS}$  = Quantity of drilling or hydraulic fracturing chemical released off-site prior to operations

$Q_S$  = Quantity of drilling or hydraulic fracturing chemical stored at intermediate locations prior to operations

$i_S$  = Portion of chemical released at intermediate storage locations

Initially a bounding estimate scenario (Tier 1) such as a catastrophic spill will be considered, where the entire amount of stored chemicals is released. In this case,  $Q_S$  will be assumed to be the maximum amounts likely to be stored, and  $i_S$  will be assumed to equal 1. The methodology for deriving  $Q_S$  values for storage at intermediate and individual wells sites is outlined in Section 4.2.2.

However, not all accidents at storage facilities would result in discharge of their entire capacity. Warehouses are expected to be bunded such that a portion, if not all of a spill will be contained on site. Accordingly, in Tier 2 more realistic volumes for values of  $i_S$  of less than 1 will be considered to reflect industry practices in spill prevention and losses from intermediate storage sites.

In Tier 3, a probability will be introduced as described in Section 3.5. However, only those spills, which are likely to exceed containment capacity, would need to be considered further.

### 3.5.3. Use exposure equations

#### 3.5.3.1. Release from mishandling of chemicals on site immediately prior to use

Chemicals are used in drilling and hydraulic fracturing. The mishandling of these chemicals, leading to leaks, overflows, and well blowouts prior to or during use at the well may lead to environmental exposure. The amount of exposure may be quantified using Release Equation 3. The methodology will be similar to that described for mishandling of chemicals at intermediate storage facilities (above), excepting that the maximum amounts would be limited to one well, the containment measures are expected to be more limited and the probabilities of a spill are likely to be different. To differentiate this value from the quantity released from storage, the variables will be denoted as  $Q_{xUP}$ ,  $Q_U$  and  $i_S$  for the chemicals released prior to operations (quantity of drilling or hydraulic fracturing chemical released on site prior to operations, the quantity of drilling or hydraulic fracturing chemical on site prior to operations and the portion of on-site fluids discharged prior to injection, respectively (where  $Q_{xUP} = Q_U \times i_S$ )). The methodology for deriving  $Q_U$  values prior to use at individual wells sites is outlined in Section 4.2.3.

#### 3.5.3.2. Release from mishandling of chemicals immediately subsequent to use

Once chemicals have been used in drilling or hydraulic fracturing a portion of them will return to the surface in the drilling or flowback water. In addition, flowback water will include any geogenics mobilised by the hydraulic fracturing process. The mishandling of these chemicals arising from leaks and overflows subsequent to use at the well may lead to environmental exposure. Although there may be losses of chemical prior to use this will only occur occasionally and is likely to be small in comparison with the total amount. Accordingly, this will not be taken into account. The amount of exposure may be quantified using Release Equation 4:

$$Q_{xUS} = [Q_U \times i_{UR} \times i_{US}] \quad \text{[Release Equation 4]}$$

Where:

$Q_{xUS}$  = Quantity of drilling or hydraulic fracturing chemical released subsequent to operations but excluding intentional disposal

$Q_U$  = Quantity of drilling or hydraulic fracturing chemical on site prior to operations

$i_{UR}$  = Portion of drilling or hydraulic fracturing chemical returned from the well

$i_{US}$  = Portion of chemical (unintentionally) released subsequent to injection

Using a tiered approach, the initial bounding estimate scenario (Tier 1), such as a catastrophic dam failure (single well site only), will be considered. In this scenario, the entire amount of temporarily stored flowback and produced water containing an amount equivalent to the amount transported to the site will be considered. For the purposes of establishing a Tier 1 upper bound estimate, it will be assumed that none of the chemical remains in the coal seam and all is returned to the surface ( $i_{UR} = 1$ ). If geogenics were included in the assessment (which is not the case in this instance),  $Q_{xUS}$  would represent the quantity mobilised rather than the quantity of drilling and hydraulic fracturing chemical on site prior to operations see also Release Equation 7. The methodology for deriving  $Q_U$  values after use is outlined in Section 4.2.3.

The likelihood that an incident at a well site would result in discharge of the entire amount of flowback and produced water, containing drilling and fracturing chemicals, is thought to be remarkably low. Incidents such as dam overflows, leaks through pond walls or leaking pipes are more likely. There may also be some containment measures to mitigate exposure from some of these routes. Accordingly, for the Tier 2 assessment more realistic volumes for values of  $i_{US}$  of less than one, will be considered to reflect industry practices in spill prevention and losses from well-sites. In addition, depending on evidence available more realistic values for  $i_{UR}$  will be used (excepting geogenics). In Tier 3, a probability of spillages at well sites will be introduced as described in Section 3.5. If chemicals are transported by tanker truck to nearby treatment facilities instead of using pipelines as described below, then the probability of a spill occurring may be calculated using Release Equation 2, divided by 2 (as only one journey is made).

### 3.5.4. Waste disposal exposure equations

#### 3.5.4.1. Fluids

Used drilling fluids can be re-used to the extent practicable for other drilling operations. Otherwise, they require disposal, which may involve treatment before disposal. Therefore, exposure due to disposal may be represented by Release Equation 5:

$$Q_{xW} = [Q_U \times i_{UR}] \times (i_{AM} \times i_{AMR} + i_{UAM}) \quad [\text{Release Equation 5}]$$

Where:

$Q_{xW}$  = Contaminant volume from wastewater disposal per well

$Q_U$  = Quantity of drilling and hydraulic fracturing chemical

$i_{UR}$  = Portion of drilling and fracturing fluid returned from the well (takes into account losses down well and degradation of fluid)

$i_{AM}$  = Portion of wastewater treated / amended and released

$i_{AMR}$  = Portion of contaminants released after treatment

$i_{UAM}$  = Portion of wastewater not treated (unamended)

Currently there is limited information on re-use, treatment and waste disposal of drilling fluids other than what has already been mentioned in Section 2.2.4.

#### 3.5.4.2. Flowback and produced waters

Flowback and produced water containing chemicals is transported (often by pipeline) to nearby storage facilities for treatment. The quantity of contaminant released from individual well sites is the amount introduced to the well site allowing for losses down the well. Again small losses from spills will be ignored. The quantity of chemicals in the flowback and produced water may be represented by Release Equation 6:

$$Q_{xWCP} = [Q_U \times i_{UR}] \quad [\text{Release Equation 6}]$$

Where:

$Q_{xWCP}$  = Contaminant quantity in wastewater per well

$i_{UR}$  = Portion of drilling and fracturing fluid returned from the well (takes into account losses down well and degradation of fluid)

If geogenics were included in the assessment (which is not the case in this instance),  $Q_{xWCP}$  would simply equal the quantity of geogenic chemicals released during fracturing and production. This may be represented by Release Equation 7:

$$Q_{xWCP} = Q_{GEO} \quad [\text{Release Equation 7}]$$

It must be noted that  $Q_{xWCP}$ , relates to the amount of chemical released from the well site to treatment storage facilities and not to the environment. Where measured concentrations for geogenic chemicals exist,  $Q_{GEO}$  may be calculated by multiplying the concentration of geogenic chemicals by the volume of water released from the well. Inflow to the storage facilities prior to treatment will come from many wells and the quantity of chemicals in the storage dams is the sum of all of the wells, which feed into the dam. The quantity of stored water in the dams may be represented by Release Equation 8:

$$Q_{xWtot} = \sum_i^n Q_{xWCP_i} \quad [\text{Release Equation 8}]$$

Where:

$Q_{xWtot}$  = Total contaminant quantity in stored wastewater from multiple wells

$Q_{xWCP_i}$  = Contaminant quantity in wastewater from each well

The stored quantity of water containing contaminants may then be released for use in various uses such as aquaculture, dust suppression, irrigation, or stored indefinitely in evaporation ponds either with or without treatment. The portion of the wastewater treated ( $i_{AMR}$ ) will have some of the contaminants removed with the remaining amount  $i_{AMR}$  released. A portion of untreated water ( $i_{UAM}$ ) may conceivably also be directly released, such as following a high intensity rainfall event. Generally single uses will involve either treated ( $i_{UAM} = 1$ ) or untreated ( $i_{UAM} = 1$ ), rather than a mixture of both. The quantity of chemical released may be represented by Release Equation 9:

$$Q_{xWD} = Q_{xWtot} \times (i_{AM} \times i_{AMR} + i_{UAM}) \quad [\text{Release Equation 9}]$$

Where:

$Q_{xWD}$  = Total contaminant released from waste disposal activities

The tiered approach in this is scenario is relatively simple as initially (Tier 1) all of the wastewater was considered untreated. In Tier 2, a more realistic split of treated and untreated portions may be considered. The quantity of contaminants released will be dependent on the contaminant and the treatment. It will be critical to understand the various treatments available and their efficacy in contaminant removal. Probability of release does not need to be considered in Tier 3 as the release is always intentional (i.e. probability = 1).

Releases from dams may be considered a special case of this scenario as the release is accidental. Accordingly, the probability may be considered as described in Section 3.5.1. For dams containing untreated water, the value for  $i_{UAM}$  is 1 and for  $i_{AM}$  it is 0. Dams containing treated water may be represented by the corollary of this statement.

### 3.5.5. Residue

During the treatment of wastewater, a residue such as brine or a precipitate will be produced. The quantity of contaminant present will be dependent on the various treatments available and their efficacy in contaminant removal. The quantity of contaminant in the residue will simply be the portion of the contaminant from the stored water ( $Q_x$ ) that is not in the treated

wastewater ( $Q_{xWD}$ ). The quantity of contaminant in the residue may be represented by Release Equation 10:

$$Q_{xWR} = Q_{xWtot} - Q_{xWD} \quad [\text{Release Equation 10}]$$

Where:

$Q_{xWR}$  = Total contaminant contained in residual brine or precipitate

The calculations for brine and solid waste containing contaminants will need further consideration, dependent on the disposal method. Currently disposal options for waste concentrates include indefinite storage, disposal to the ocean, injection into aquifers and landfill (of solids). See Section 2.2.4 above for details. Pond liners and clean-up spill kits are not included in this consideration, as they will be disposed of to landfill and not result in direct exposure to the environment (see Section 2.3).

### 3.5.6. Removal pathways

There may be losses of chemical during the chemical lifecycle that are not well accounted for in the above considerations. For example, chemicals may degrade (decompose to simpler chemicals), or volatilise to air or partition to sediment in storage facilities for flowback and produced water before their release into the environment.

Biological and inorganic chemical degradation are the only pathways by which a given chemical can be removed from the chemical lifecycle permanently. The predominant mechanisms by which chemicals degrade in the environment include hydrolysis, photolysis and biotic pathways, as noted in Section 2.4.4. Although these degradation pathways exist for chemicals during each stage of the chemical lifecycle, the conditions in which they will occur during coal seam gas extraction activities will be highly modified from those encountered in the natural environment. For example, microorganism populations and thus biodegradation in storage dams may be reduced compared to natural surface waters due to the presence of lining (which separates the water from soil micro-organisms) and hydraulic fracturing and geogenic chemicals (which may be toxic to microorganism populations). Accordingly, studies relating to removal of chemicals in the environment may not be able to be extrapolated to chemicals when in the coal seam gas lifecycle.

Some pathways such as partitioning to sediment during storage in ponds, and mechanical separation or flocculation during water treatment may remove chemicals from one waste stream (thereby transferring it into another waste stream), which may reduce the contaminants' concentration in the water column resulting in reduced exposure to the environmental compartment from the releases of this water. However, these chemicals are not destroyed and may simply be held in storage indefinitely in storage ponds or approved waste facilities. Therefore, these chemicals may still be released to the environment through processes such as slow leakage through dam linings or dam failure.

Volatilisation represents a transport pathway from the aquatic compartment to the air. This may result in a loss of chemicals from their lifecycle, such as removal from flowback and produced water in storage facilities. An estimation of this loss may be made based on a static system (no exchange of air or water) according to Henry's Law (Exposure Equation 19). However, as discussed in Sections 2.4.3 and 2.5.4 the atmospheric compartment is dynamic and losses are not readily calculated.

All of these pathways have the potential to reduce the quantity of contaminant in the release environment. However, they will not be considered in the precautionary estimates of quantity used in Tiers 1 and 2 of the risk assessment. Expert judgement will be required to determine

the extent to which the representation of chemical fate pathways in the environment (Section 3.4) is appropriate for determining removal in Tier 3.

## 4 Inputs

### 4.1. Introduction

This Section describes the general methodology used to derive selected inputs for the mathematical expressions outlined in Section 3. Current available data and assumptions were used to provide an input value. However, it must be recognised that these assumptions need to be reviewed periodically as industry practices will change over time. Accordingly, any values used in this assessment should be regarded as current estimates and may change as new information is obtained. Unless otherwise stated, the values used will be those obtained from a literature review by the Department of the Environment and Energy (DoEE 2017a), or reported by industry via the industry survey (NICNAS 2017b). Relevant input values are provided in Appendix D (Table D.1, Table D.2, and Table D.3).

### 4.2. Release

The approach to calculating the released quantities of chemicals used in drilling and hydraulic fracturing is described in Section 3.5. The approach requires inputs for the quantity of drilling or hydraulic fracturing chemical, transported ( $Q_T$ ), stored ( $Q_S$ ) and used on site ( $Q_U$ ). From this, the quantities released from waste disposal ( $Q_{xWD}$ ) and the amount remaining in the brine or precipitate ( $Q_{xWR}$ ) may be derived. For transport accidents, a specific equation has been used to define the probability ( $P_T$ ), of such accidents. This will require input values for the number of truck accidents per year ( $N_C$ ), the total number of shipments (by truck) per year ( $N_S$ ) and the proportion of trucks that crash resulting in a spill ( $i_{TC}$ ).

#### 4.2.1. Transport

Transport considers the quantity of chemicals moved to intermediate storage sites (denoted  $Q_{Ti}$ ) and then required quantities to individual well sites (denoted  $Q_{Tw}$ ). This is determined by the volume of drilling and hydraulic fracturing formulations transported ( $V_T$ ) multiplied by the concentration of drilling or hydraulic fracturing chemical in the formulation ( $C_F$ ) as represented by Input Equation 1:

**Input equation 1:**

$$Q_T = V_T \times C_F \quad [\text{Input Equation 1}]$$

Where:

$Q_T$  = Quantity of drilling or hydraulic fracturing chemical transported

$V_T$  = Volume of drilling and hydraulic fracturing formulations transported

$C_F$  = Concentration of drilling or hydraulic fracturing chemical in the formulation

Where the chemical is a solid the value of  $V_T$  is considered as a mass (in kg) and  $C_F$  is considered in percentage by weight (w/w). The quantities of each reported formulated product used in the Australian coal seam gas industry were obtained from a literature review by the Department of the Environment and Energy (DoEE 2017a), or reported by industry via the industry survey (NICNAS 2017b). These formulated products, which may either comprise a single chemical or mixture, are transported in 2 to 25 kg containers or up to 10 000 kg bulk bags for solids and in 20 L containers, 206 L drums or 500 to 1 000 L totes for liquids.



Information gathered during the industry survey under the National Coal Seam Gas Chemicals Assessment (NICNAS 2017b) details the individual chemicals and their concentration in most, but not all, formulations. These data comprise the base dataset that will be used for the risk assessment. The individual chemical concentrations in formulated products on delivery to the site ( $C_F$ ) used in the risk assessment are provided in Appendix D (Table D.1 and Table D.2).

To derive individual chemical quantities transported to intermediate storage sites ( $Q_{Ti}$ ) for the bounding estimate (Tier 1) assessment model developed in Section 3 it will be assumed that the volume of formulated product transported ( $V_T$ ) is equal to truck capacity and that the individual chemical is transported at its maximum reported concentration in any formulation ( $C_{Fmax}$ ) in the industry survey.

When refining the scenario (Tier 2), individual chemical quantity ( $Q_{Ti}$ ) may be cross-referenced with formulation quantity data to provide a more realistic upper limit for chemicals used in low volumes, with the assumed container sizes adjusted accordingly. For example, if a chemical is present in formulations imported in quantities below the maximum container size, then the assumed container size or number of container units may be adjusted to be below the import quantity. Additionally, the number of container units actually carried on a truck may be reconsidered to take into account that the import volume may be used in disperse geographic locations and thus would be stored at a number of intermediate storage sites. However, there is currently no available data relating individual chemicals or formulated products to locations of use.

Probability of transport accidents ( $P_T$ ) may be introduced in the final refinement (Tier 3) of the scenario. Input values for  $N_C$ ,  $N_S$  and  $i_{TC}$  may be based on available data, such as (Driscoll 2011).

Transport to individual well sites includes both formulated products and intermediate blends. The chemical quantities ( $Q_{Tw}$ ) transported are expected to be greater than or equal to the amounts required for the number of hydraulic fracturing operations at one well site. The derivation for the chemical quantity used at a single well site,  $Q_U$ , is described in Section 4.2.3. The chemical quantity available for release during transport to the well site is  $Q_U$  rounded up to the most appropriate container size based on the quantity of formulated product required. This can be determined, assuming that no intermediate blending occurs, by assuming the volume of formulated product delivered to the site ( $V_T$ ) is equivalent to the quantity required for use divided by the concentration as expressed by Input Equation 2:

$$V_T = \frac{Q_U}{C_{Fmax}} \quad [\text{Input Equation 2}]$$

Where:

$Q_U$  = Quantity of drilling or hydraulic fracturing chemical at a single well site

$V_T$  = Volume of drilling and hydraulic fracturing formulated product delivered to the site

$C_{Fmax}$  = Maximum concentration of drilling or hydraulic fracturing chemical in the formulation

The value of  $V_T$  can then be used to estimate the likely quantity and container sizes on a single truck. Where rounding up to the most appropriate container size is less than 10% of  $V_T$ , an additional container may be assumed.

Table 4.1 provides the likely volume inputs to determine chemical quantity. The concentrations ( $C_F$ ) will be determined from the industry survey (NICNAS 2017b).



Table 4.1 Likely inputs used at each assessment tier to determine chemical quantity released during transport to intermediate storage facilities

Exposure scenario	Tier 1	Tier 2	Tier 3
Transport to intermediate sites	$V_T$ = Truck capacity (10 000 kg or L)	$V_T$ = Multiples of container unit sizes such as 206 L, 25 kg, 1 000 L totes, depending on operational requirements	Values for $N_c$ , $N_s$ and $i_{TC}$ will require further evaluation

The quantity of chemicals transported from well sites to nearby storage facilities (see Table 4.1), will be derived from Release Equation 1 and Release Equation 2 (Section 3.5.1) which are dependent on other input values. Accordingly no new input values need to be considered.

#### 4.2.2. Storage

Intermediate sites are expected to hold multiple truck volumes of chemical although the precise quantities are not known. The quantity ( $Q_s$ ) of drilling and hydraulic fracturing chemicals stored at intermediate storage sites is determined by similar methods as expressed in Input Equation 2 except that the volume stored of drilling and hydraulic fracturing formulations is  $V_s$ .

For assessment of individual chemical quantities ( $Q_s$ ) as part of the Tier 1 model developed in Section 3.4.2, it is assumed that the volumes or mass imported, manufactured, or acquired locally of all formulations are delivered to one intermediate site. In this case, the value of  $V_s$  is equivalent to the formulation quantities provided in NICNAS (2017b), reproduced in part in Appendix D (Table D.3). Although the formulation quantities apply to multiple companies for finite time periods (two years for hydraulic fracturing chemicals), information on the number of intermediate sites or the number of wells that an intermediate site serves is not available. Furthermore, there may be single chemicals and formulated products that are restricted in use to one area. In this case, the quantity  $V_s$  may be delivered to one intermediate site only. At Tier 2, more realistic quantities may be considered based on distribution of chemical use across multiple sites where this information is available.

#### 4.2.3. Industrial use

At the well site, drilling and hydraulic fracturing chemicals may be stored as formulations, intermediate blends and final process fluids. However, the quantity ( $Q_U$ ) of chemicals available for calculating the release at the well site will be the same regardless of the release medium.  $Q_U$  is determined from the volume ( $V_U$ ) and concentration ( $C_F$ ) of hydraulic fracturing or drilling fluids using Input Equation 2 (see Section 4.2.1) but changing the suffix letters such as  $Q_T = V_U \times C_F$ .

The NICNAS (2017b) report also provides quantities of injected formulation fluid and individual chemicals per operation for a subset of the product formulations and chemicals. For chemicals without quantity data,  $Q_U$  can be determined using Input Equation 3 and the chemical concentration ranges in the final diluted process fluid ( $C_D$ ), which is provided in NICNAS (2017b).  $V_s$  is assumed to be up to 1.1 ML (DoEE 2017a):

$$Q_u = C_D \times V_s \quad [\text{Input Equation 3}]$$

Where:

$Q_u$  = Quantity of drilling or hydraulic fracturing chemical at a single well site

$V_s$  = Total volume injected into the well during hydraulic fracturing operations

$C_D$  = Chemical concentration ranges in the final diluted process fluid injected into the well during hydraulic fracturing operations

The way in which information was provided in NICNAS (2017b) requires that the quantities of drilling chemicals be calculated in different ways. Where possible, a method using an assumed  $V_s$  equivalent to the drilling fluid system volume (159 000 to 318 000 L), the range of concentrations ( $C_D$ ) provided in NICNAS (2017b), and in a confidential attachment (not included) was used (given the expected variable use of chemicals across different wells). Otherwise, it was assumed that the national import volume divided by 82 (the number of wells to which this volume applies) (DoEE 2017a) gives the volumes per well, and this value multiplied by the concentration range gives the amount of chemical. This is considered less reliable as it assumes uniform use across all 82 wells.

The individual concentrations of industrial chemicals used in drilling and hydraulic fracturing ( $C_D$ ) to be used in the risk assessment are provided in Appendix D (Table D.1 and Table D.2).

#### **4.2.4. Disposal**

##### **4.2.4.1. Drilling fluids**

Currently there are no direct input values for  $Q_{xwD}$  (total contaminant released from waste disposal activities). Methods were explored to derive this value from other known values. Values exist for the quantity (bounding estimate =  $Q_u$ ) of returned drilling chemicals to the pre-injection sump of up to 0.3 ML. However, another value identified in the literature review was 2.6 ML. In addition to the highly variable volumes of returned drilling fluid, no values exist for concentration. Consequently, there does not appear to be a current method to derive  $Q_{wD}$  based on the available data.

##### **4.2.4.2. Hydraulic fracturing fluids**

No input values are required for individual well values as these will be derived values. However, an estimate is required for the number of wells feeding a storage pond ( $n$ ) to calculate  $Q_{xwtot}$  (total contaminant quantity in stored wastewater) for multiple wells using Release Equation 8. This may be estimated as follows.

The capacity of storage ponds is variable, with a maximum dam capacity of 840 ML identified (Coffey Environments 2012). With up to 1.1 ML fluid used in hydraulic fracturing operations and with a 110% return volume (DoEE 2017a), this could theoretically hold flowback and produced water from  $(840/1.1 =) 760$  operations. However, it is much more likely that the specific chemical inputs from each individual well will be highly variable, where the input of a certain chemical is attributed to only a few of the wells. In addition, hydraulic fracturing may be undertaken at only a percentage of the wells (e.g. in the Surat Basin up to 40% to 60% of wells reportedly require hydraulic fracturing [DoEE 2017a]). The number of wells ( $n$ ) feeding a dam is not well known. However, it will be dependent on the ratio of wells in an area which require hydraulic fracturing in comparison with the total number of wells.

#### **4.3. Receiving environment**

##### **4.3.1. Aquatic**

The volume of the aquatic receiving environment is given by Exposure Equation 3. This requires inputs for  $V_{environmental}$ ,  $V_{contaminated}$  and  $V_{uncontaminated}$ . The variables for Exposure Equation 3 at each Tier are shown in Table 4.2.

Table 4.2 Variables for Exposure Equation 3 at each Tier

Variable	Tier 1	Tier 2	Tier 3
$V_{environmental}$	First order stream. Default volume of 1 500 m <sup>3</sup> or disposal outfall flow	Bioregional definitions for low flow conditions observed selected streams	Accounts for variability of the bioregional stream
$V_{contaminated}$	Volumes as defined by release scenario. Further refinement is not required	Volumes as defined by release scenario. Further refinement is not required	Volumes as defined by release scenario. Further refinement is not required
$V_{uncontaminated}$	No uncontaminated volume. Default volume of 0 m <sup>3</sup>	Potential for uncontaminated water sources considered	Potential for uncontaminated water sources considered

### 4.3.2. Soil

To determine the concentration of a chemical in soil (Exposure Equation 4), data pertaining to the area over which the contaminant is spread, the depth to which it penetrates and the density of the soil is required.

#### 4.3.2.1. Area

Produced water may be deliberately applied to soil through irrigation and dust suppression. The area under consideration may be chosen based on agricultural practices for irrigation provided the rate of application (in quantity per area) is known. In Australia, the default value is application of 1 metre of water per hectare per year (EPHC 2009a), equivalent to 10 ML of water over one hectare per year.

For dust suppression, the area may be limited to that of interest (e.g. roads, work sites, etc.). Effective dust suppression may be achieved at spray rates of 1.4 to 4.9 L/m<sup>2</sup> with preferred rates between 3 to 3.5 L/m<sup>2</sup> (Soilbond 2006; Dust Control Solutions 2009). The actual rate of application will depend on operational requirements and lower rates are used for slope erosion control and stockpile dust control, while higher rates are recommended for trails, paths and unpaved roads with light to heavy traffic (Minova 2011). The use of water only for dust suppression is expected to require higher spray volumes per unit area compared to the use of a dust suppression treatment (DuPont 2007).

Spills will need to be treated differently as they spread out based on the nature of the spill and properties of the fluid and soil. The model is described in Exposure Equation 5.

Once the spill no longer spreads, infiltration will continue until all surface liquid has infiltrated. The applicability of this model in determining the area over which a spill spreads, including data availability, was evaluated during the risk assessment.

#### 4.3.2.2. Depth

Estimates of depth of soil to which the contaminant penetrates have been made by US EPA (2005a, 2005b) and EPHC (2009b), according to soil types and use. Values under consideration for the depth of soil to which contaminants may penetrate are shown in Table 4.3.

Table 4.3 Values under consideration for the depth of soil to which contaminants may penetrate

Source	Value	Comment
US EPA (2005a)	1 cm	Untilled non-agricultural
US EPA (2005b)	2 cm	Untilled
US EPA (2005a)	10 cm	Tilled minimum
EPHC (2009b)	15 cm	Australian default value
US EPA (2005a)	20 cm	Tilled maximum

In the case of spills, the depth of penetration may be limited as the spill may spread over a large area. For spills, it is expected that the depth to which penetration occurs may be determined by the volume of soil required to absorb the liquid. This may be determined from the soil moisture and the soil saturation point (Maximum Water Holding Capacity). The depth of penetration may then be calculated from the volume of soil required to absorb the liquid divided by the area over which the spill spreads, as described by exposure Equation 5 and Exposure Equation 6.

#### 4.3.2.3. Density

Several publications (US EPA 2005a and 2005b; EPHC 2009a) have separately determined default values for the density of soil based on averages of measured values. Values under consideration for density of soil are shown in Table 4.4.

Table 4.4 Values under consideration for the density of soil

Source	Value	Comment
US EPA (2005b)	1 500 kg/m <sup>3</sup>	Average of measured data range of bulk density between 830 to 1 840 kg/m <sup>3</sup>
EPHC (2009a)	1 500 kg/m <sup>3</sup>	Australian default value

#### 4.3.2.4. Accumulation

For accumulation of contaminants in soil, the timing between applications is required. The timing between applications may be determined by irrigation requirements and some guidance is provided by EPHC (2009a and 2009b). For dust suppression, industry practice may provide information on timing, but these practices are currently unknown. The rate of degradation of chemicals can be measured, but if inadequate data is available it can be modelled (at higher tier assessment levels, not in Tier 1) (Section 3.4.6). Where the values are provided as half-lives (in days), the rate constant (in days<sup>-1</sup>) may be calculated from the well-known relationship for first order kinetics  $DT_{50} = \ln_2/k$ , which may be rearranged to  $k = \ln_2/DT_{50}$ .

### 4.4. Environmental fate

#### 4.4.1. Runoff

Several model inputs independent of the chemical are required for the quantification of runoff (Exposure Equation 9). Values used in Exposure Equation 9 to determine the percentage of contaminant in runoff water are shown in Table 4.5.

Table 4.5 Values used in Exposure Equation 9 to determine the percentage of contaminant in runoff water

Variable	Tier 1	Tier 2	Tier 3
$\Psi$	Precipitation (mm/day). To be determined. Values between 1 and 100 mm based on DSEWPaC (2009) and OECD (2000).	Bounding estimate rainfall based on regional data.	The probability of rain exceeding a certain value based on regional data will be used as described in Section 3.4.2.
R	Runoff (mm/day). To be determined by the methodology described above (Section 3.4.2) and verified using ANRA (2001).	Regional data on soil types and hence curve numbers.	Allow for variability of soil types within region.
Heterogeneity factor	Bounding estimate value of 1.	Refined values 0.5 to 1 based on Dunne and Black (1970), Kuhn and Zhu (2008).	No change
Retention factor	Depending on release scenario 0.5 to 1 (Linders et al. 2000; Willis et al. 1994).	No change	No change
Transport-suspended contaminant	0 for contaminants with water solubility $\geq 1$ mg/L (Grover 1989).	% suspended sediment as calculated by Release Equation 4.	No change
Slope	20% or 12.5% depending on scenario.	9%, 7.5% or 5% (Balmer and Frey 2001; OECD 2000) and available GIS data.	Allow for variability of slopes within region.
Buffer	Default Value 1 (No effect).	No change	No change
DT50soil	Assume no degradation (DT50 = $\infty$ ; k = 0).	Use bounding estimate DT50 value.	Use more likely DT50 values, such as the geometric mean or 95 <sup>th</sup> percentile.
Koc	Assume no affinity for soil (Koc = 0).	Use bounding estimate Koc value.	Use more likely Koc values, such as the geometric mean or 95 <sup>th</sup> percentile.
OC	0.3% for agricultural uses (ANRA 2001). Non-agricultural uses will require further investigation.	Regional data on soil types and organic carbon values.	Allow for variability of soil types within region.

## 5 Model validation

### 5.1. Validation data

The validation of the models developed during the risk assessment, to estimate the PECs, involves comparison of calculated PEC values with measured environmental concentration data. This requires identification of case study data, which is representative of the scenario being modelled. The data must be assessed for quality and appropriateness to the model before use. In particular the data needs to be assessed for sampling bias (intentional or unintentional), sensitivity of the measurements for environmental concentrations, and adequate consideration of system components that may critically affect the values obtained.

A brief search of coal seam gas company reports reveals that appropriate case studies may be available to validate some of the calculations. One potential case study measured environmental concentrations in contaminated soil following release of flowback and / or produced water from an intake pipe at a reverse osmosis plant (Golder Associates 2012). The suitability of this data was assessed during the risk assessment to determine if it could be used for validating the calculations. A case study with measured environmental concentrations in surface waters has not been identified.

### 5.2. Confidence and sensitivity of data inputs

The literature review conducted by the Department of the Environment (DoEE 2017a) as part of the National Coal Seam Gas Chemicals Assessment project raised the issues of model uncertainty and sensitivity of data inputs. Some uncertainty is irreducible. Therefore an evaluation of uncertainty and confidence in the predictive modelling is desirable. Data choice also critically affects the validity of the model outputs. It is therefore vital that the overall sensitivity of the assessment to key parameter values and assumptions is evaluated, as described in the report *Environmental risks associated with surface handling of chemicals used in coal seam gas extraction* (DoEE 2017b).

#### 5.2.1. Confidence in models

Bounding estimate scenarios predict the highest possible environmental concentration and may over-predict due to the compounding of conservative estimates. As the tiered approach only refines model inputs if a risk is identified from bounding estimate scenarios, any uncertainty in the model will be included in the consideration of bounding estimate scenarios. This increases the confidence in the modelled results.

#### 5.2.2. Sensitivity

Sensitivity analysis is a method of determining which inputs for a model are important. It involves a systematic, pragmatic technique to understand how model outputs are dependent on variability and uncertainty of the input factors, thereby identifying what is 'driving' the output estimates (US EPA 2001). There is a wide array of analytical methods that may be referred to as sensitivity analyses, some of which are very simple and intuitive. Initially the relative contributions of exposure pathways were analysed either by qualitative analysis or by one variable at a time analysis, keeping other variables constant. For major pathways the equations used for predicting release or environmental concentrations were analysed by partial derivatives to obtain a sensitivity ratio. Where the relationship between input and the output parameters is non-linear (e.g. operations such as powers and square roots), then an

analysis may use various statistical inputs. Example statistical inputs include the mean, the 95<sup>th</sup> percentile, the maximum and the minimum.



## 6 Summary

The scope of this report is limited to surface-to-surface exposures. Infiltration and volatilisation are only examined as a mechanism for losses from the soil and water compartments. The extent of exposure of the shallow groundwater compartment is not considered in this report and is discussed in Mallants et al. (2017c).

This report describes the lifecycle of chemicals used in coal seam gas extraction, the potential points of release during the lifecycle, and the chemical fate pathways to selected aquatic receptors in the receiving environments. Potential sources of surface-related contamination have been reviewed and are reported in NICNAS (2017a), DoEE (2017a), Jeffrey et al. (2017), Apte et al. (2017), and Mallants et al. (2017a). Additional information about potential sources of contamination and their release are reported in NICNAS (2017b). Potential risks of contamination of soil and groundwater from chemical use associated within each of the different phases involved in developing a coal seam gas well field have been summarised by CSIRO (Mallants et al. 2017a) and are further conceptualised by Mallants et al. (2017b). In this report the stages of transport, storage, use, and disposal were considered for their potential releases. The potential release points considered in this report include:

- spills or leaks
- leakage from storage impoundments
- improperly constructed well casings
- poor recovery of fluids injected during the hydraulic fracturing process
- intentional surface applications of treated or untreated produced water for beneficial use (Mallants et al. 2017b)
- Once chemicals entered the receiving environment, their fate pathways were conceptualised to inform predictions of the transfer or transformation of contaminants between different environmental compartments.

Eight potential points of release at a working site were conceptualised, based on where in the lifecycle an accidental spill of chemical or intentional release to the environment may occur. They were:

- transport of chemicals
- storage of chemicals at intermediate warehouse sites
- storage of chemicals at individual well sites
- use of chemicals at individual well sites
- management of coal seam gas waste fluids (i.e. flowback and produced waters)
- storage of coal seam gas waste fluids
- irrigation
- dust suppression.

Figure 6.1 shows the eight potential points of release at a working site.

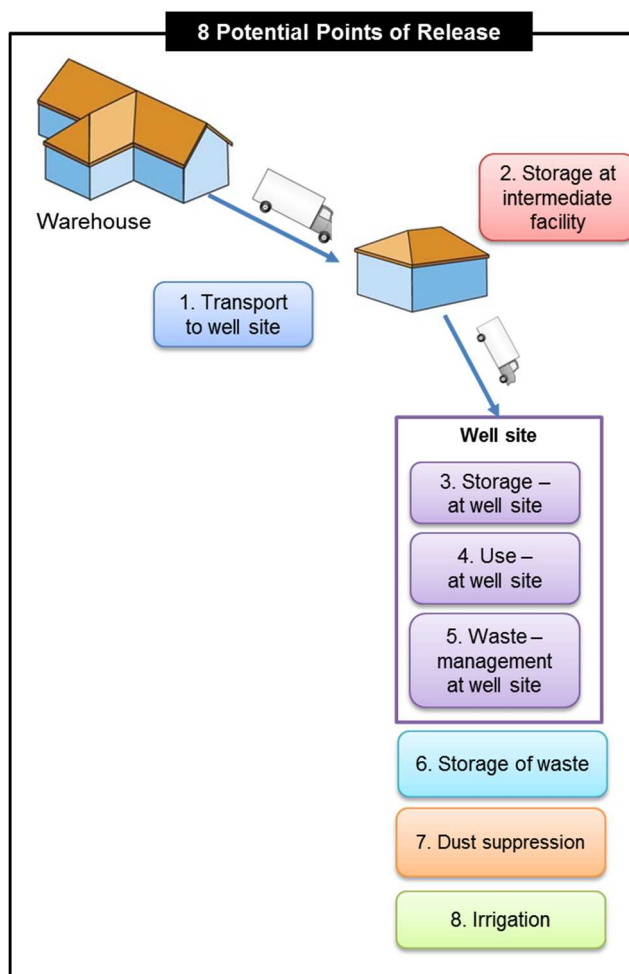


Figure 6.1 The eight conceptualised potential points of release from the chemical lifecycle within a coal seam gas working site

Mathematical expressions were developed and / or adapted to estimate chemical concentrations for the different components of the environmental exposure modelling (the chemical quantity, the points of release, the chemical fate pathways, and the receiving environmental receptors). The mathematical expressions to determine the chemical concentrations from the points of release are based on a mass balance approach such that all releases or losses of chemicals are accounted for. In general, the environmental concentration in receiving environments is calculated using a simple ratio of the quantity of chemical in the environment to the volume of the receiving environment. Generally, the system is assumed to be static (i.e. no changes in quantity or volume), but dynamic systems can be used where required to simulate more realistic scenarios, such as those in higher tier assessments.

The main transport and fate pathways for chemicals are considered to be runoff, volatilisation, deposition, sedimentation, infiltration and transport in shallow groundwater, and degradation. The focus of the environmental risk assessment is runoff to surface receptors. The runoff calculations can estimate the chemical concentration at the edge of the field in a tiered manner. In the first tier, the movement of chemical in runoff water is considered only in relation to the ratio of runoff water to precipitation and independently of the chemical's properties such as degradation or adsorption to soil. In Tier 2, chemical properties are considered as well as more realistic soil properties. Tier 3 examines the probability of runoff occurring. Other fate pathways likely to be minor are only considered in a single Tier.

For the aquatic receiving environment, the volume selected to estimate the chemical environmental concentration ( $PEC_{\text{aquatic}}$ ) is also tiered. Initially (Tier 1) the largest amount of chemical and a hypothetical low flow first order stream in the vicinity of coal seam gas extraction activities are considered. This also acts as a surrogate for the effects of releases from multiple wells. In Tier 2, considerations include more realistic environmentally important streams in a region, with measured flow data and where appropriate, contributions to the water volume from uncontaminated areas. Tier 3 considers chemical fate and behaviour in the receiving environments and incorporates natural variability of the water volumes.

For soil, the area over which the flowback or produced water is spread and the depth to which it penetrates may be regarded as the soil receiving environment. Tier 1 considers the shallowest depth, while Tier 2 considers more environmentally representative depths. Tier 3 considers variability in soil types and losses of chemical via leaching to depths no longer considered part of the surface environment.

Overall, the approach to develop the conceptual exposure scenarios was:

- based on mass balance
- tiered – refinement of initially conservative (upper bound) scenarios to more realistic ones occurred only if unacceptable risk is shown in the lower tier assessment
- precautionary – considers the bounding estimate in each tier
- able to act as a surrogate for multiple releases in the bounding estimate scenarios.

The quantity of chemical present in each of the stages of the lifecycle was estimated from the industry survey (NICNAS 2017b) and literature reviews [including DoEE (2017a)]. A total of 113 industrial chemicals were identified for consideration in the environmental risk assessment. Some of the limitations identified in this report, which will impact on the validation of the models to be used for the risk assessment and the results produced, include data availability for key areas such as chemical information (e.g. concentrations for points of release), and site information (e.g. storage capacity, sources and number of spills per year). However, these data gaps were addressed using generic assumptions and alternative methods to derive the necessary inputs for the predictive modelling.

Table 6.1 Summary of release scenarios

Lifecycle stage	Point of release	Medium	Volume
Transport			
Intermediate site	Truck accident	Neat chemical and formulated product	Proportion of national import volume
Well site	Truck accident	Neat chemical and formulated product	Site specific
Storage			
Intermediate site	Container spills/leaks	Neat chemical and formulated product Intermediate blend	Proportion of national import volume
Well site	Container spills/leaks	Neat chemical and formulated product Process fluid	Site specific
Use			
Well site	Blending spills	Process fluid	Site specific
Well site	Pipe leaks	Process fluid	Site specific
Well site	Well blowouts	Process fluid	Site specific
Well site	Dam overflow	Flowback and produced water and returned drilling fluid	110%
Disposal			
Well site	Reuse and disposal	Drilling fluid	As required
Well site	Collection	Flowback and produced water	Maximum permitted rate
Well site	Dam overflow	Flowback and produced water	Unknown
Well site	Surface water discharge	Flowback and produced water	As required
Well site	Environmental flows	Flowback and produced water	As required
Well site	Aquaculture	Flowback and produced water	As required
Well site	Irrigation	Flowback and produced water	Maximum permitted rate
Well site	Dust suppression	Flowback and produced water	Maximum permitted rate
Well site	Indefinite storage/evaporation	Flowback and produced water Brine	Unknown
Well site	Brine pond	Flowback and produced water Brine	Unknown
Well site	Managed aquifer recharge	Flowback and produced water	Unknown

Lifecycle stage	Point of release	Medium	Volume
Well site	Industrial re-use	Flowback and produced water	Unknown

Table 6.2 Summary of chemical fate and partitioning mechanisms leading to exposure to a secondary receiving environment

Primary receiving environment	Pathway	Secondary receiving environment	Equation
Water	Instantaneous	N/A	Exposure Equation 1 to 6 Release Equation 9
	Dilution	Water	Exposure Equation 1 to 6 Release Equation 9
	Sedimentation	Sediment	Exposure Equations 21 and 22
Soil	Instantaneous	N/A	Exposure Equation 7 to 9 Release Equation 1 to 4
	Deposition	Soil	Exposure Equation 7 to 9 Release Equation 9
	Runoff	Soil	Exposure Equation 5 to 7 Release Equation 1 to 10
	Runoff	Water	Exposure Equation 9 to 14 Release Equation 1 to 10
	Infiltration	Groundwater	Not in scope
Air	Volatilisation	Air	Exposure Equations 19 and 20

N/A = not applicable.

## 7 References

- Adgate, JL, Goldstein, BD and McKenzie, LM 2014, 'Potential public health hazards, exposures and health effects from unconventional natural gas development', *Environmental Science and Technology*, 48(15), pp. 8307-8320.
- ANRA 2001, Australian agriculture assessment, National Land And Water Resources Audit, Land and Water Australia on behalf of the Commonwealth of Australia, Appendix 2. (Australian Natural Resources Atlas) ISBN: 0 642 37121 0. Accessed: 26 May 2009 at [http://www.anra.gov.au/topics/agriculture/pubs/national/agriculture\\_asris.html](http://www.anra.gov.au/topics/agriculture/pubs/national/agriculture_asris.html)
- Apte, SC, Kookana, RS, Batley, GE and Williams, M (2017a, *Literature review: Geogenic contaminants associated with the hydraulic fracturing of coal seams*, report prepared by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- APVMA 2010, *Agricultural manual of requirements and guidelines - Ag MORAG*, Volume 3 Data, Part 7 Environment, 3rd edn, Australian Pesticides and Veterinary Medicines Authority, Canberra.
- Atkins, PW 1986, *Physical chemistry*, 3rd edn, Oxford University Press, Oxford.
- Balmer, ME and Frey, S 2001, *Swiss final report on the validation of OECD pesticide aquatic risk indicators*, FAW, Swiss Federal Research Station for Fruit- Growing, Viticulture and Horticulture and Swiss Federal Institute for Environmental Science and Technology, Zurich.
- Coffey Environments 2012, *Surat gas project: environmental impact statement*, report to Arrow Energy Pty Ltd, Coffey Environments, Brisbane.
- Cook, RU and Doornkamp, JC 1973, *Geomorphology in environmental management – an introduction*, Oxford University Press, Oxford.
- CSIRO undated, Monitoring off-site transport of nutrients, sediment and pesticides from cherries, apples and grapes in the Mount Lofty Ranges. Accessed: 30 March 2009 at <http://www.clw.csiro.au/publications/projects/MtLoftyMonitoring.pdf>
- DEEDI 2011, *Code of practice for constructing and abandoning coal seam gas wells in Queensland*, Department of Employment, Economic Development and Innovation, Queensland Government, Brisbane.
- DEHP 2014, *Coal Seam Gas / Liquid Natural Gas Compliance Plan, 2012-13 End of year report*, Report prepared by the Department of the Environment and Heritage Protection (DEHP), Queensland Government, Brisbane.
- Driscoll, OP 2011, *Major accident investigation report*, National Truck Accident Research Centre, Brisbane.
- DSEWPac 2009, *Background document to Chemical Assessment Section's reviewed approach to runoff*, June 2009, unpublished report prepared by the Australian Government Department of Sustainability, Environment, Water Population and Communities, Canberra.
- DSEWPac 2012, *Diuron review volume 2 of 4 supplemental environmental assessment report runoff risk assessment*, report to the Australian Pesticides and Veterinary Medicines Authority, Australian Government Department of Sustainability, Environment, Water Population and Communities, Canberra.

- DoEE 2017a, *Literature review: environmental risks from coal seam gas operations*, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS) of the Department of the Environment and Energy as part of the National Assessment Of Chemicals Associated With Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- DoEE 2017b, *Environmental risks associated with surface handling of chemicals used in coal seam gas extraction*, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS) of the Department of the Environment and Energy as part of the National Assessment Of Chemicals Associated With Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- Dunne, T and Black, RD 1970, 'Partial area contributions to storm runoff in a small New England watershed', *Water Resources Research*, vol. 6(5), pp. 1296-1311.
- DuPont 2007, DuPont case study: reducing dust emissions from unsealed roads and open areas, DuPont, Macquarie Park.
- Dust Control Solutions 2009, *Dust control solutions, EC-46: dust suppressant*. Accessed: [http://www.dustcontrol.com.au/products/EC\\_46.html](http://www.dustcontrol.com.au/products/EC_46.html)
- EC 2003, Technical guidance document on risk assessment in support of commission directive 93/67/EEC on risk assessment for new notified substances; commission regulation (EC) no 1488/94 on risk assessment for existing substances; directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. Part II. European Communities.
- EC 2012, *Toxicity and Assessment of Chemical Mixtures*, SCHER, SCENIHR, and SCCS opinion, November and December, 2012. European Commission, Brussels. Accessed: [http://ec.europa.eu/health/scientific\\_committees/environmental\\_risks/docs/scher\\_o\\_155.pdf](http://ec.europa.eu/health/scientific_committees/environmental_risks/docs/scher_o_155.pdf)
- EPHC 2009a, *Environmental risk assessment guidance manual for industrial chemicals*, report prepared by Lee-Steere, C, Australian Environment Agency Pty Ltd for Environment Protection and Heritage Council, Canberra. Accessed: [www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals](http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals)
- EPHC 2009b, *Environmental risk assessment guidance manual for agriculture and veterinary chemicals*, report prepared by Lee-Steere, C, Australian Environment Agency Pty Ltd for Environment Protection and Heritage Council, Canberra. Accessed: [www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals](http://www.scew.gov.au/resource/chemical-risk-assessment-guidance-manuals)
- Flewelling, SA and Sharma, M 2014, 'Constraints on Upward Migration of Hydraulic Fracturing Fluid and Brine', *Groundwater*, Jan-Feb 2014, 52(1), pp. 9-19.
- FOCUS 2006, Guidance document on estimating persistence and degradation kinetics from environmental fate studies on pesticides in EU registration. Accessed: 10 September 2009 at <http://focus.jrc.ec.europa.eu/dk/>
- Golder Associates 2012, *Bibblwindi Water Treatment Facility soil investigation*, report for Santos Limited, Golder Associates.
- Groat CG and Grimshaw TW 2012, *Fact-Based Regulation for Environmental Protection in Shale Gas Development*, Report prepared by The Energy Institute, University of Texas, Austin, USA.
- Grover, R ed. 1989, *Environmental chemistry of herbicides*, vol. 1, CRC Press Inc, Florida.
- Jeffrey, R, Wu, B, Bunger, A, Zhang, X, Chen, Z, Kear, J and Kasperczyk, D 2017, *Literature review: Hydraulic fracture growth and well integrity*, Project report prepared by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) as part of



- the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- Keller, JM and Simmons, CS 2005, *The influence of selected liquid and soil properties on the propagation of spills over flat permeable surfaces in the Pacific Northwest*, report for the U.S. Department of Energy.
- Kookana, RS 1998, 'Pesticide fate and behaviour in Australian soils in relation to contamination and management of soil and water: a review', *Australian Journal of Soil Research*, vol. 1998(36), pp. 715-64.
- Kortenkamp, A, Backhaus, T and Faust, M 2009, *State of the art report on mixture toxicity – final report*, report to the European Commission, DG Environment.
- Kuhn, NJ and Zhu, H 2008, GIS-based modeling of runoff source areas and pathways, *Geographica Helvetica*.
- Lin, SH, Sahai, R and Eyring, H 1971, 'Kinetics of heterogeneous chemical reactions: a theoretical model for the accumulation of pesticides in soil', *Proceedings of the National Academy of Science*, vol. 68(4), pp. 777-780.
- Linders, J, Mensink, G, Stephenson, D, Wauchope, D and Racke, E 2000, 'Foliar interception and retention values after pesticide application, 'A proposal for standardized values for environmental risk assessment (Technical report)', *Pure Applied Chemistry*, vol. 72(11), pp. 2199-2218.
- LMC 2011, *OASIS Catalogic vol. 5.10.9*, Laboratory of Mathematical Chemistry, Bourgas University, Bourgas, Bulgaria.
- Lutz, W 1984, *Berechnung von hochwasserabflüssen unter anwendung von gebietskenngrößen*, Mitteilung Nr. 24, des Instituts für Hydrologie und Wasserwirtschaft, Universität Karlsruhe, Karlsruhe.
- Mallants, D, Bekele, E, Schmid, W, Miotlinski, K and Bristow, K 2017a, *Literature review: Identification of potential pathways to shallow groundwater of fluids associated with hydraulic fracturing*, prepared by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- Mallants, D, Bekele, E, Schmid, W and Miotlinski, K 2017b, *Human and environmental exposure conceptualisation: Soil to shallow groundwater pathways*, report prepared by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- Mallants, D, Bekele, E, Schmid, W, Miotlinski, K and Gerke, K 2017c, *Human and environmental exposure assessment: Soil to shallow groundwater pathways – A study of predicted environmental concentrations*, report prepared by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- Maniak, U 1988, *Hydrologie und wasserwirtschaft*, Springer-Verlag, Berlin.
- Merz, R 2008, Regionalisierung von ereigniskenngrößen wiener Mitteilungen Band 197: methoden der hydrologischen Regionalisierung.
- Minova 2011, *RD10 Dust control: product data*. Accessed at: <http://www.minova.com.au/assets/RD10-Dust-Control-PDS-31.8.11.pdf>

- Myers, T 2012, 'Potential contaminant pathways from hydraulically fractured shale to aquifers', *Groundwater*, 50(6), pp. 872-882.
- NRCS 1986, *Urban hydrology for small watersheds, technical release 55*, Natural Resources Conservation Service, United States Department of Agriculture Conservation Engineering Division.
- NICNAS 2017a, *Literature review: Human health implications and regulation*, Project report prepared by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- NICNAS 2017b, *Identification of chemicals associated with coal seam gas extraction in Australia*, project report prepared by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- NICNAS 2017c, *Human health risks associated with surface handling of chemicals used in coal seam gas extraction*, Project report prepared by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.
- OECD 2000, Report of the OECD Pesticide Aquatic Risk Indicators Expert Group for phase 1 of the Aquatic Risk Indicators Project annex 2, Organisation for Economic Co-operation and Development.
- Probst, M, Berenzen, N, Lentzen-Godding, A and Schulz, R 2005, 'Scenario-based simulation of runoff-related pesticide entries into small streams on a landscape level', *Ecotoxicology and Environmental Safety*, vol. 62(2), pp. 145-159.
- Rozell, DJ and Reaven, SJ 2012, 'Water pollution risk associated with natural gas extraction from the Marcellus Shale', *Risk Analysis*, vol. 32, pp. 1382-1393.
- Rutovitz J, Harris SM, Kuruppu N and Dunstan C 2011, *Drilling down: Coal seam gas – a background paper*, Report prepared by the Institute for Sustainable Futures, University of Technology Sydney, pp. 1-83. Accessed: 13 June 2014 at <http://cfsites1.uts.edu.au/find/isf/publications/rutovitzetal2011sydneycoalseamgasbkgs.pdf>
- Soilbond 2006, *Dust control guidelines: technical data sheet TDS 003*. Accessed: 2 May 2006, [soilbond.com.au/downloads/soilbond-dust-control.pdf](http://soilbond.com.au/downloads/soilbond-dust-control.pdf)
- SPDEFTP 2003, *Environmental flow determination of the Steels, Pauls and Dixons Creek catchments: part B – final recommendations*. Accessed: 3 August 2013 at [http://www.melbournwater.com.au/content/library/rivers\\_and\\_creeks/stream\\_flow\\_management/stream\\_flow\\_reports/environmental\\_flow\\_determination\\_recommendations.pdf](http://www.melbournwater.com.au/content/library/rivers_and_creeks/stream_flow_management/stream_flow_reports/environmental_flow_determination_recommendations.pdf)
- 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*, 275, pp.37-54. Accessed: <http://dx.doi.org/10.1016/j.jhazmat.2014.04.040>
- The Royal Society and The Royal Academy of Engineering 2012, *Shale gas extraction in the UK: a review of hydraulic fracturing*, Report prepared by The Royal Society and The Royal Academy of Engineering, UK. Accessed: 12 June 2014 at <http://www.raeng.org.uk/shale>

- US EPA 2014, Framework for Ecological Risk Assessment. Accessed: [http://www.epa.gov/oppefed1/ecorisk\\_ders/index.htm#framework](http://www.epa.gov/oppefed1/ecorisk_ders/index.htm#framework)
- US EPA 1992, *Guidelines for exposure assessment*, Federal Register 57(104):22888-22938. EPA/600/Z-92/001 May 1992, US Environmental Protection Agency, Washington, DC.
- US EPA 2001, *FIRST: a screening model to estimate pesticide concentrations in drinking water*, May 1. Accessed: 17 September 2008 at <http://www.epa.gov/oppefed1/models/water/models4.htm>
- US EPA 2004, *Refined (level II) terrestrial and aquatic models for probabilistic and ecological assessment of pesticides March 30 - April 2*. Accessed: 22 July 2014 at [http://www.epa.gov/oppefed1/ecorisk/ecorisk\\_fifrasap.htm](http://www.epa.gov/oppefed1/ecorisk/ecorisk_fifrasap.htm)
- US EPA 2005a, *Human health risk assessment protocol, Chapter 5: Estimating media concentrations*. Accessed: 1 August 2013 at <http://www.epa.gov/wastes/hazard/tsd/td/combust/riskvol.htm>
- US EPA 2005b, *Appendix B: Estimating media concentration equations and variable values (sections B-4-15 to B4-4-25)*. Accessed: 1 August 2013 at <http://www.epa.gov/wastes/hazard/tsd/td/combust/finalmact/ssra/05hhrapapb.pdf>
- Vidic RD, Brantley SL, Vandenbossche JM, Yoxtheimer D and Abad JD 2013, 'Impact of shale gas development on regional water quality', *Science*, 340(6134). Accessed: <http://science.sciencemag.org/content/340/6134/1235009>
- Willis, GH, McDowell, L, Smith, S and Southwick, LM 1994, 'Permethrin and sulprofos washoff from cotton plants as a function of time between application and Initial rainfall', *Journal of Environmental Quality*, vol. 23(1), pp. 96-100.

## Appendix A – Curve numbers

The curve numbers (CN) developed by NRCS (1986) did not specifically address the influence of soil moisture on runoff. To better account for this influence, as reported by Merz (2008), Maniak (1988) and Lutz (1984) developed the following equations to describe the effect of rainfall occurring during the growing season (April to October in the Northern Hemisphere).

The CN for soil is modified dependent on the rainfall occurring in the previous five days (during the growing season). If the sum of the rainfall occurring in the previous five days is less than 30 mm then the modified CN value  $CN_1$  is given by Equation A1:

$$CN_1 = \frac{CN}{2.334 - 0.01334 \times CN} \quad \text{[Equation A1]}$$

Where:

$CN$  = the value reported by NRCS (1986).

If the rainfall total is between 30 and 50 mm then  $CN_2 = CN$ . If the rainfall total exceeds 50 mm then  $CN_3$  is described by Equation A2:

$$CN_3 = \frac{CN}{0.4036 + 0.0059 \times CN} \quad \text{[Equation A1]}$$

## **Appendix B – Confidential business information**

This appendix contained Confidential business information (CBI) and has been removed from this public reporting version of the report.

## Appendix C – Composition of five hydraulic fracturing fluid mixtures

Table C.1 Composition of five hydraulic fracturing fluid mixtures

CAS RN	Chemical name	Conc. after final dilution prior to injection (g/L)
	<b><i>YF120LG – typical crosslink gel</i></b>	
10043-35-3	Boric acid (H <sub>3</sub> BO <sub>3</sub> )	0.1532
10377-60-3	Nitric acid, magnesium salt	0.0069
14464-46-1	Cristobalite (SiO <sub>2</sub> )	0.0007
14807-96-6	Talc (Mg <sub>3</sub> H <sub>2</sub> (SiO <sub>3</sub> ) <sub>4</sub> )	0.0006
14808-60-7	Quartz (SiO <sub>2</sub> )	89.3494
25038-72-6	2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene	0.0152
26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	0.0037
2682-20-4	3-Isothiazolone, 2-methyl-	0.0011
497-19-8	Carbonic acid, disodium salt	0.316
533-96-0	Carbonic acid, sodium salt (2:3)	0.8317
64-19-7	Acetic acid	0.0709
67-63-0	2-Propanol	0.0134
75-57-0	Methanaminium, N,N,N-trimethyl-, chloride	1.2733
7631-86-9	Silica	0.0059
7727-54-0	Peroxydisulfuric acid ((HO) <sub>3</sub> SOOSO <sub>3</sub> H), diammonium salt	0.4521
7786-30-3	Magnesium chloride (MgCl <sub>2</sub> )	0.0034
9000-30-0	Guar gum	2.171
91053-39-3	Kieselguhr, calcined	0.0344
	<b><i>20# Linear Gel – Batch Mix</i></b>	
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	0.04125
7447-40-7	Potassium chloride (KCl)	22.9629
7681-52-9	Hypochlorous acid, sodium salt	0.05775
9000-30-0	Guar gum	2.39653
9025-56-3	Hemicellulase	0.03636
	<b><i>20# Crosslink Gel – Batch Mix</i></b>	

CAS RN	Chemical name	Conc. after final dilution prior to injection (g/L)
1310-73-2	Sodium hydroxide (NaOH)	0.1375
10043-35-3	Boric acid (H <sub>3</sub> BO <sub>3</sub> )	0.216
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	0.04125
7447-40-7	Potassium chloride (KCl)	22.9629
7681-52-9	Hypochlorous acid, sodium salt	0.05775
7772-98-7	Thiosulfuric acid (H <sub>2</sub> S <sub>2</sub> O <sub>3</sub> ), disodium salt	0.175
9000-30-0	Guar gum	2.39653
9025-56-3	Hemicellulase	0.03636
	<b>20# Crosslink Gel – On-the-Fly</b>	
107-21-1	1,2-Ethenediol	0.496
1303-96-4	Borax (Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O)	0.372
1310-73-2	Sodium hydroxide (Na(OH))	0.124
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	0.04125
7447-40-7	Potassium chloride (KCl)	22.9629
7681-52-9	Hypochlorous acid, sodium salt	0.05775
9000-30-0	Guar gum	2.6
9025-56-3	Hemicellulase	0.03636
	<b>Treated water</b>	
90622-53-0	Alkanes, C <sub>12-26</sub> branched and linear	206
26062-79-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer	1.302
55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	0.04125
64-19-7	Acetic acid	0.525
7447-40-7	Potassium chloride (KCl)	22.9629
75-57-0	Methanaminium, N,N,N-trimethyl-, chloride	0.612
7647-01-0	Hydrochloric acid	0.0525
7681-52-9	Hypochlorous acid, sodium salt	0.05775
77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	1.76504
9000-70-8	Gelatins	2.99566



## Appendix D – Exposure assessment input values

A critical step in exposure assessment is to identify chemicals that may potentially be released into the environment as a result of coal seam gas extraction in Australia. To determine the quantity of a chemical released at various stages of the chemical life-cycle, its concentration in release media including soil, water, and air must be known. Ideally, representative chemical compositions and concentrations in all release media would be readily available. This would allow quantification of exposure during the risk assessment. The identified release media relevant to coal seam gas extraction include single chemicals, formulated products, intermediate blends, process fluids, and waste products (i.e. drilling muds, flowback and water produced) and concentrates (brine).

The data gathered in the report on the *Identification of chemicals associated with coal seam gas extraction in Australia* (NICNAS 2017b) is the primary source of chemical composition and concentration information included in this report. The quantity of chemical present in each of the stages of the lifecycle was estimated from the industry survey (NICNAS 2017b) and literature reviews [including DoEE (2017a)]. A total of 113 industrial chemicals were identified for consideration in the environmental risk assessment.

For industrial chemicals used in drilling, the industry survey identified single chemicals and formulated products that were expected to be used over a 19 week period at 82 wells across Australia. For industrial chemicals used in hydraulic fracturing, the industry survey identifies single chemicals and formulated products used over a two year period. The mixture composition of five hydraulic fracturing process fluids is also available (Appendix C).

The concentration of a chemical in formulated products ( $C_F$ ) is an input for estimating the quantity of chemical in Section 4.2.1. The  $C_F$  values to be used in a bounding estimates for exposure assessments are provided in Table D1 and Table D.2 for drilling and hydraulic fracturing chemicals respectively. Where a value is confidential it is reported as 'CBI' (confidential business information). The confidential values, while available to the authors during the assessment, are not included in this version of the report.

The selected bounding estimate  $C_F$  values are the maximum, upper limit of the reported range in the *Identification of chemicals associated with coal seam gas extraction in Australia* (NICNAS 2017) and the further confidential information (NICNAS pers comm., 2 April 2013). For the two drilling and 10 hydraulic fracturing chemicals without  $C_F$  data, under a bounding estimate exposure scenario it will be assumed that the chemical is brought to the site as a single undiluted chemical (i.e. not diluted by other chemicals).

The concentration of a chemical that has been diluted in process fluids ( $C_D$ ) is an input for estimating the quantity of chemical in Section 4.2. The  $C_D$  values, (rounded to three significant figures) used in the bounding estimate for exposure assessments are provided in Table D1. and Table D.2 for drilling and hydraulic fracturing chemicals, respectively. Where the maximum value is a confidential value, it is indicated as 'CBI' (confidential business information). The confidential values, while available to the authors during the assessment, are not included in this version of the report.

Table D.1 Concentration in formulated products ( $C_F$ ) and process fluids ( $C_D$ ) of industrial chemicals used in drilling

Number	CAS RN	Chemical name	$C_F$ (Formulated product, g/L or g/kg)	$C_D$ (Process fluid, g/L)
1	107-22-2	Ethanedial/glyoxal	CBI	CBI
2	111-30-8	Pentanedial/Glutaraldehyde	300	CBI
3	11138-66-2	Xanthan gum	1 000	CBI
4	1302-78-9	Bentonite	1 000	CBI
5	1303-96-4	Borax ( $\text{Na}_2(\text{B}_4\text{O}_7) \cdot 10\text{H}_2\text{O}$ )	24	CBI
6	1305-62-0	Calcium hydroxide ( $\text{Ca}(\text{OH})_2$ )	1 000	CBI
7	1310-73-2	Sodium hydroxide ( $\text{NaOH}$ )	1 000	CBI
8	1317-65-3	Limestone	> 990	CBI
9	144-55-8	Carbonic acid, monosodium salt	1 000	CBI
10	14464-46-1	Cristobalite ( $\text{SiO}_2$ )	10	CBI
11	14808-60-7	Quartz ( $\text{SiO}_2$ )	50	CBI
12	15468-32-3	Crystalline silica, tridymite	10	CBI
13	497-19-8	Carbonic acid, disodium salt	2 532	CBI
14	64-17-5	Ethanol	100	CBI
15	64742-47-8	Distillates, petroleum, hydrotreated light	600	CBI
16	67-56-1	Methanol	CBI	CBI
17	67-63-0	2-Propanol	100	10*
18	7447-40-7	Potassium chloride (KCl)	1 000	CBI
19	7727-43-7	Sulfuric acid, barium salt (1:1)	1 000	CBI
20	7757-83-7	Sulfurous acid, disodium salt	1 000	CBI
21	7758-16-9	Diphosphoric acid, disodium salt	1 000	CBI
22	7778-80-5	Sulfuric acid, dipotassium salt	1 000	CBI
23	77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	1 000	CBI
24	9000-30-0	Guar gum	CBI	CBI
25	9003-06-9	2-Propenoic acid, polymer with 2-propenamide	CBI	CBI
26	CBI	2-Ethylhexanol heavies	CBI	CBI
27	CBI	Fatty acids ester	1 000	CBI

Number	CAS RN	Chemical name	C <sub>F</sub> (Formulated product, g/L or g/kg)	C <sub>D</sub> (Process fluid, g/L)
28	CBI	Polyacrylamide/polyacrylate copolymer	950	CBI
29	CBI	Ester alcohol	CBI	CBI
30	CBI	Polymer	CBI	CBI
31	CBI	Organic sulfate	1 000*	100*
32	CBI	Organic acid salt	CBI	CBI
34	CBI	Polymer with substituted alkylacrylamide salt	CBI	CBI
35	CBI	Polymer	CBI	CBI
36	CBI	Polysaccharide	1 000	CBI
37	CBI	Natural fibres	CBI	CBI
38	n.s.	Natural fibres	CBI	CBI
39	n.s.	Natural fibres	CBI	CBI
40	n.s.	Nut hulls	CBI	CBI
42	n.s.	Polyesters	CBI	CBI
43	n.s.	Walnut hulls	1 000	CBI
44	n.s.	Wood dust	CBI	CBI
45	n.s.	Wood fibre	CBI	CBI

\* Assumed value—concentration is not available in the industry survey. n.s. = not supplied; CBI = confidential business information.

Table C.3 7.1 Concentration in formulated products (C<sub>F</sub>) and process fluids (C<sub>D</sub>) of industrial chemicals used in hydraulic fracturing fluid

Number	CASRN	Chemical name	C <sub>F</sub> (Formulated product, g/L or g/kg)	C <sub>D</sub> (Process fluid, g/L)
1	10043-35-3	Boric acid (H <sub>3</sub> BO <sub>3</sub> )	36	0.216
2	10043-52-4	Calcium chloride (CaCl <sub>2</sub> )	CBI	CBI
3	10377-60-3	Nitric acid, magnesium salt	50	0.0069
4	107-21-1	1,2-Ethenediol	496	0.496
5	108-10-1	2-Pentanone, 4-methyl-	CBI	CBI
6	111-76-2	Ethanol, 2-butoxy-	1 000*	10*
7	111-90-0	Ethanol, 2-(2-ethoxyethoxy)-	CBI	CBI

Number	CASRN	Chemical name	C <sub>F</sub> (Formulated product, g/L or g/kg)	C <sub>D</sub> (Process fluid, g/L)
8	12008-41-2	Boric acid, (H <sub>2</sub> B <sub>8</sub> O <sub>13</sub> ), disodium salt	1 000	10*
9	124-38-9	Carbon dioxide	1 000	N/A
10	1303-96-4	Borax (Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O)	372	0.372
11	1305-78-8	Calcium oxide	CBI	CBI
12	1310-73-2	Sodium hydroxide (NaOH)	1 000	CBI
13	1318-16-7	Sintered bauxite	CBI	CBI
14	141-43-5	Ethanol, 2-amino-	15	CBI
15	144-55-8	Carbonic acid, monosodium salt	1 000	CBI
16	14464-46-1	Cristobalite (SiO <sub>2</sub> )	CBI	CBI
17	14807-96-6	Talc (Mg <sub>3</sub> H <sub>2</sub> (SiO <sub>3</sub> ) <sub>4</sub> )	1 000*	0.0006
18	14808-60-7	Quartz (SiO <sub>2</sub> )	2 650	120
19	25038-72-6	2-Propenoic acid, methyl ester, polymer with 1,1-dichloroethene	1 000*	0.0152
20	26038-87-9	Boric acid (H <sub>3</sub> BO <sub>3</sub> ), compound with 2-aminoethanol	600	CBI
21	26062-79-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer	651	1.30
22	26172-55-4	3(2H)-Isothiazolone, 5-chloro-2-methyl-	1 000*	0.0037
23	2634-33-5	1,2-Benzisothiazol-3(2H)-one	CBI	CBI
24	2682-20-4	3-Isothiazolone, 2-methyl-	1 000*	0.0011
25	497-19-8	Carbonic acid, disodium salt	2 530	10* <sup>6</sup>
26	52-51-7	1,3-Propanediol, 2-bromo-2-nitro-	1 000	CBI
27	533-96-0	Carbonic acid, sodium salt (2:3)	1 000	0.8317

<sup>6</sup> The concentration reported in the industry survey (2 530 g/L) is inconsistent with the findings of the literature review that hydraulic fracturing fluids typically contains less than 3% of chemicals other than water and proppant. In addition, it is likely the chemical is a solid at the reported concentration. In the absence of reliable concentration information the assumed bounding estimate value is used.

Number	CASRN	Chemical name	C <sub>F</sub> (Formulated product, g/L or g/kg)	C <sub>D</sub> (Process fluid, g/L)
28	55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	CBI	CBI
29	56-81-5	1,2,3-Propanetriol	CBI	CBI
30	584-08-7	Carbonic acid, dipotassium salt	500	1 *
31	6381-77-7	D-Erythro-hex-2-enonic acid, gamma.-lactone, monosodium salt	1 000	10*
32	6410-41-9	2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino) sulfonyl]-2-methoxyphenyl]azo]-3-hydroxy-	CBI	CBI
33	64-17-5	Ethanol	300	CBI
34	64-19-7	Acetic acid	1 050	0.525
35	67-56-1	Methanol	100	CBI
36	67-63-0	2-Propanol	300	CBI
37	68130-15-4	Guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt	1 000	10*
38	68187-17-7	Sulfuric acid, mono-C6-10-alkyl esters, ammonium salts	1 000 *	10*
39	68439-45-2	Alcohols, C6-12, ethoxylated	1 000 *	10*
40	68647-72-3	Terpenes and terpenoids, orange oil	300	CBI
41	7447-40-7	Potassium chloride (KCl)	1 990	23.0
42	75-57-0	Methanaminium, N,N,N-trimethyl-, chloride	612	1.27
43	7631-86-9	Silica	CBI	CBI
44	7647-01-0	Hydrochloric acid	600	CBI
45	7647-14-5	Sodium chloride (NaCl)	10 000	CBI
46	7681-52-9	Hypochlorous acid, sodium salt	300	CBI
47	7727-37-9	Nitrogen	1 000	N/A
48	7727-54-0	Peroxydisulfuric acid ((HO) <sub>3</sub> SOOSO <sub>3</sub> H), diammonium salt	1 000	0.452

Number	CASRN	Chemical name	C <sub>F</sub> (Formulated product, g/L or g/kg)	C <sub>D</sub> (Process fluid, g/L)
49	7757-82-6	Sulfuric acid, disodium salt	CBI	CBI
50	7757-83-7	Sulfurous acid, disodium salt	CBI	CBI
51	7758-19-2	Chlorous acid, sodium salt	100	10*
52	7772-98-7	Thiosulfuric acid (H <sub>2</sub> S <sub>2</sub> O <sub>3</sub> ), disodium salt	600	0.175
53	7775-27-1	Peroxydisulfuric acid ((HO) <sub>3</sub> SOOSO <sub>3</sub> H), disodium salt	1 000	10*
54	7783-20-2	Sulfuric acid, diammonium salt	300	10*
55	7786-30-3	Magnesium chloride (MgCl <sub>2</sub> )	1 000*	0.0034
56	77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	1 000	1.77
57	81741-28-8	Phosphonium, tributyltetradecyl-, chloride	100	10*
58	9000-30-0	Guar gum	1 050	2.6
59	9000-70-8	Gelatins	1 000	3.00
60	9003-05-8	2-Propenamide, homopolymer	600	10*
61	9004-62-0	Cellulose, 2-hydroxyethyl ether	1 000	10*
62	9012-54-8	Cellulase	150	10*
63	9025-56-3	Hemicellulase	1 200	0.0364
64	90622-53-0	Alkanes, C12-26 branched and linear	520	10* <sup>7</sup>
65	91053-39-3	Kieselguhr, calcined	1 000*	0.0344
66	CBI	Enzyme	CBI	CBI
67	CBI	Amine salt	CBI	CBI
68	CBI	Inner salt of alkyl amines	CBI	CBI
69	CBI	Ethoxylated fatty acid I	CBI	CBI
70	CBI	Ethoxylated fatty acid II	CBI	CBI
71	CBI	Ethoxylated fatty acid III	CBI	CBI

<sup>7</sup> The concentration reported in the industry survey of 206 g/L is inconsistent with the findings of the literature review that hydraulic fracturing fluids typically contains less 3% of chemicals other than water and proppant. In the absence of reliable concentration information the assumed bounding estimate value is used.

Number	CASRN	Chemical name	C <sub>F</sub> (Formulated product, g/L or g/kg)	C <sub>D</sub> (Process fluid, g/L)
72	CBI	Terpenes and terpenoids	CBI	CBI
73	CBI	Quaternary amine	CBI	CBI
74	CBI	Polyamine	CBI	CBI
75	n.s.	Walnut hulls	1000	CBI

\* Assumed value—concentration is not available in the industry survey; n.s. = not supplied; CBI = confidential business information.

All available concentration data for drilling fluids are confidential. The selected bounding estimate C<sub>D</sub> value for each drilling chemical is the maximum value in the confidential attachment (not included) to the industry survey (NICNAS 2017b). To specify a bounding estimate exposure scenario for the three drilling chemicals without reported concentration data, it was assumed that the formulated product containing the chemical is diluted by a factor of 0.1 when used in drilling fluids<sup>8</sup>.

The selected bounding estimate C<sub>D</sub> value for each hydraulic fracturing chemical is the maximum of the upper limit of the range reported by NICNAS (2017b), and further, unpublished, confidential information. Two chemicals, nitrogen and carbon dioxide, are expected to be used in coal seam gas stimulation techniques other than hydraulic fracturing (i.e. gas displacement). Given that these are natural components of the atmosphere, environmental exposure from the use of these gases in hydraulic fracturing is not expected. Hence, C<sub>D</sub> values are not derived. Under a bounding estimate exposure scenario, C<sub>D</sub> will be assumed to equal 1%w/v (or 10 g/L)<sup>9</sup> for the other hydraulic fracturing chemicals with no data.

The composition of some of the formulated products is confidential. The available results based on non-confidential information are provided in Table D.3. The confidential results, while available to the authors during the assessment, are not included in this version of the report.

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<sup>8</sup> The dilution factor for 40 drilling chemicals with reported concentrations in both formulated products and process fluids were calculated using the maximum values. The results ranged between 0.0007 and 0.24. The majority of chemicals (37) had a dilution factor of less than 0.043. The three chemicals for which an estimate is required are considered unlikely to be used in a similar way (i.e. have the same function) as those chemicals with a dilution factor above 0.043 based on structural considerations. A dilution factor of 0.1 is selected as a conservative estimate.

<sup>9</sup> The reported maximum concentrations of chemicals in hydraulic fracturing process fluids range from 10-5 to 23 g/L (excluding proppants and other exceptions as noted in **Error! Reference source not found.**). The concentrations of 52 of 53 hydraulic fracturing chemicals are below 1%w/v, or 10 g/L, in process fluids. A concentration of 10 g/L is adopted as a bounding estimate value for a hydraulic fracturing chemical in process fluids.



Table D.3 Concentration of chemicals in formulated products used in hydraulic fracturing and calculated maximum quantity of chemical used in the Australian coal seam gas industry (based on the reported quantity of formulated product imported or locally manufactured)

Number	Formulation	CASRN	Chemical name	C <sub>F</sub> (g/L)	Individual chemical import quantity (QT <sub>i</sub> )
1	Boric Acid 3.6%	10043-35-3	Boric acid (H <sub>3</sub> BO <sub>3</sub> )	36	288 L
2	XLW-10A	107-21-1	1,2-Ethanediol	400	915 L
3	XLW-10A	1303-96-4	Borax (Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O)	300	686 L
4	Sodium Hydroxide 10%	1310-73-2	Sodium hydroxide (NaOH)	1 000	4 000 L
5	XLW-10A	1310-73-2	Sodium hydroxide (NaOH)	100	229 L
6	WG-19	141-43-5	Ethanol, 2-amino-	15	10 kg
7	Magnacide-575	55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	600	499 L
8	Tolcide PS75	55566-30-8	Phosphonium, tetrakis(hydroxymethyl)-, sulfate (2:1) (salt)	750	58 L
9	GasPerm 1100	64-17-5	Ethanol	300	3 179 L
10	GasPerm 1100	67-56-1	Methanol	100	1 060 L
11	GasPerm 1000	67-63-0	2-Propanol	300	31 L
12	GasPerm 1100	67-63-0	2-Propanol	100	1 060 L
13	GasPerm 1000	68647-72-3	Terpenes and terpenoids, orange oil	300	31 L
14	GasPerm 1100	68647-72-3	Terpenes and terpenoids, orange oil	50	530 L
15	ClayTreat-3C	75-57-0	Methanaminium, N,N,N-trimethyl-, chloride	600	240 L
16	Hydrochloric Acid, 22 baume	7647-01-0	Hydrochloric acid	382	3 832 L
17	HC-2	7647-14-5	Sodium chloride (NaCl)	100	75 L
18	HpH Breaker	7647-14-5	Sodium chloride (NaCl)	300	716 L
19	Sodium Hypochlorite 12.5%	7681-52-9	Hypochlorous acid, sodium salt	1 000	12 000 L

Number	Formulation	CASRN	Chemical name	C <sub>F</sub> (g/L)	Individual chemical import quantity (QT <sub>i</sub> )
20	GS-1L	7772-98-7	Thiosulfuric acid (H <sub>2</sub> S <sub>2</sub> O <sub>3</sub> ), disodium salt	600	120 L
21	Citric Acid	77-92-9	1,2,3-Propanetricarboxylic acid, 2-hydroxy-	1 000	25 kg
22	GW-3	9000-30-0	Guar gum	990	4 950 kg
23	WG-36	9000-30-0	Guar gum	1 000	93 628 kg
24	GLFC-5	9000-30-0	Guar gum	500	1 500 L
25	GW-3	9000-30-0	Guar gum	900	4 500 kg
26	WG-19	9000-30-0	Guar gum	1 000	687 kg
27	Gelatine	9000-70-8	Gelatins	1 000	50 kg
28	GBW-12CD	9025-56-3	Hemicellulase	1 000	69 L
29	GLFC-5	90622-53-0	Alkanes, C12-26 branched and linear	500	1 500 L
30	HC-2	n.s.	Inner salt of alkyl amines	300	225 L