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

Technical report number 8

Human and environmental exposure conceptualisation: Soil to shallow groundwater pathways

This report was prepared by CSIRO

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Reports in this series

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Foreword

Purpose of the Assessment

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

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

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

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

Australia's regulatory framework

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

Approach

Technical experts from the National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the Commonwealth Scientific and Industrial Research Organisation (CSIRO), and the Department of the Environment 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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[1] See Mallants et al., 2017a; Jeffrey et al., 2017a; Adgate et al., 2014; Flewelling and Sharma, 2014; DEHP, 2014; Stringfellow et al., 2014; Groat and Grimshaw, 2012; Vidic et al., 2013; Myers, 2012; Rozell and Reaven, 2012; The Royal Society and The Royal Academy of Engineering, 2012; Rutovitz et al., 2011.

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. The project is not an assessment of the risks of any particular site where coal seam gas extraction is taking place or proposed.

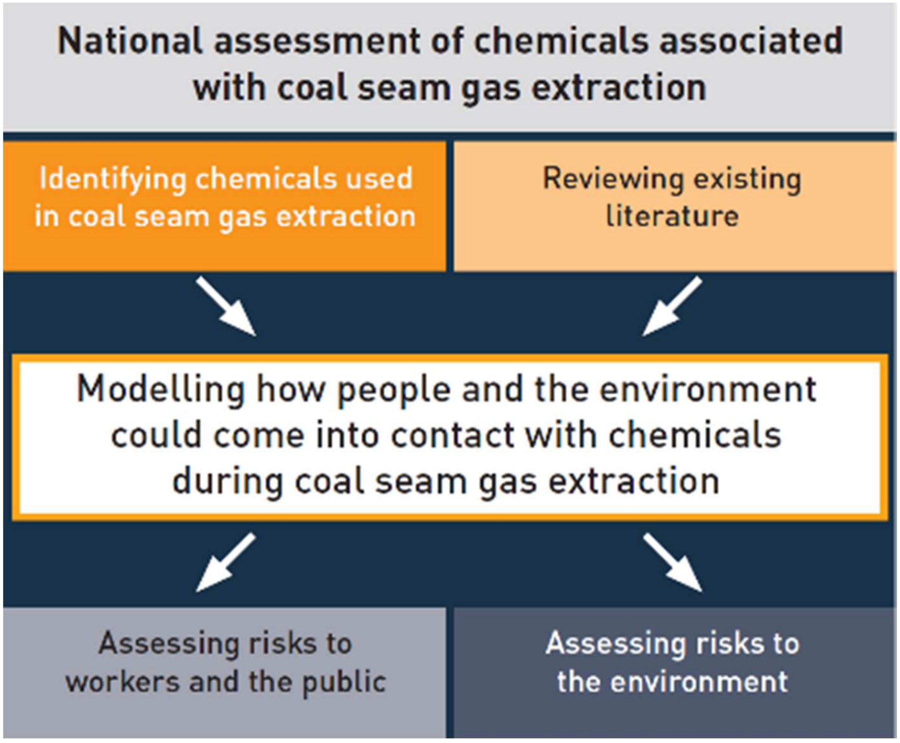


Figure F.1 Steps in the assessment

Collaborators

The Australian Government Department of the Environment 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: *Human and environmental exposure conceptualisation: Soil to shallow groundwater pathways*

This report is part of the 'modelling of 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 soil, shallow groundwater, wetlands and streams, resulting from spills and leaks at the land surface. These models incorporate the best current understanding of the complex soil-shallow groundwater system 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.

The conceptualisation process considered pathways of chemical transport through soil and shallow groundwater, with soil pore water and shallow drinking water wells as receiving environments. Wetlands and streams were also considered as receiving environments for the downstream discharge of shallow groundwater at the surface.

Chemical concentrations calculated in these receiving environments provided input to the exposure assessment calculations for human receptors.

This study developed the first tier of a multi-tiered approach for the soil and groundwater pathway. In this Tier 1 approach solute transport in soil and groundwater neglects chemical interactions between contaminants and the solid phases (minerals and organic matter) and biogeochemical transformation. A Tier 1 assessment also uses generic, high-end estimates of the range of site properties influencing chemical transport. In reality, chemical attenuation is likely to play a much more prominent role and distances between source and receiving environments will be much longer than those considered in this study. The approach adopted is therefore conservative and may overestimate chemical concentrations.

The conceptual model for the unsaturated zone accounts for different solute sources at the land surface and their characteristics. The fate pathways, for which detailed conceptual models have been developed here, included spills from small containers (a few litres) to large totes (several thousands of litres), and short-term and long-term leakage from untreated water storage ponds (containing flowback and / or produced water) under conditions of normal operation.

The usefulness of a Tier 1 assessment with a generic groundwater model is limited when the results need to be representative of a broad set of hydrogeological conditions. In the context of the National Coal Seam Gas Chemicals Assessment, such a broad set of hydrogeological conditions is informed by the priority bioregions agreed by the Australian Government. Rather than developing several region-specific groundwater models – a complex undertaking that is not necessary in a Tier 1 approach aimed at delivering high end estimates – a limited set of groundwater flow models in a single sub-bioregion were developed. These models were then used as a basis for more detailed groundwater transport calculations to derive precautionary, high end predictions of environmental concentrations. The predicted environmental concentrations developed using these models were generalised for use in a range of bioregions where coal seam gas extraction is taking place (or proposed) in Australia. The predicted environmental concentrations were not specific to any particular site where coal seam gas extraction is taking place or proposed.

A comprehensive approach to ensuring confidence in the numerical modelling process and the reporting of its outputs is also presented. There is a high degree of confidence in the conceptualisation of the pathways to estimate exposure concentrations. As a result, the near-surface groundwater transport pathway for chemicals can be utilised directly to inform the human health risk assessment processes being conducted by the National Coal Seam Gas Chemicals Assessment.

Abbreviations

General abbreviations	Description
AE	Arrow Energy
ANZECC	Australian and New Zealand Environmental and Conservation Council
ARMCANZ	Agriculture and Resource Management Council of Australia and New Zealand
CBAS	Chemical and Biotechnology Assessment Section of the Department of the Environment
CSIRO	Commonwealth Scientific and Industrial Research Organisation
DEHP	Queensland Department of Environment and Heritage Protection
DERM	Queensland Department of Environment and Resource Management (now known as the Department of Natural Resources and Mines – DNRM)
DoE	Department of the Environment
DTI	New South Wales Department of Trade and Investment
ET	Evapotranspiration
HFF	Hydraulic fracturing fluid
LHS	Latin Hypercube Sampling
LOC	Levels of concern
MC	Monte Carlo
NCM	Namoi Catchment Model
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
PDF	Probability density function
PEC	Predicted environmental concentration
PRCC	Partial rank correlation coefficient
SANTOS	South Australia Northern Territory Oil Search
RQ	Risk quotient
US EPA	United States Environmental Protection Agency

Symbols

Units or symbols	Description
α	Dispersivity (m)
c	Solute concentration in the water phase (mg/L)
C_s	Solubility limit (mg/L)
D	Hydrodynamic dispersion coefficient (m^2/s)
D_p	Pore-water diffusion coefficient, also referred to as molecular diffusion coefficient (m^2/s)
DF	Dilution factor (-)
K_d	Distribution coefficient, also referred to as soil-water partition coefficient (L/kg)
ℓ	Mualem pore connectivity parameter [-]
α, n, m	Curve shape parameters of the van Genuchten model (m^{-1}, -, -)
η	Total porosity (cm^3/cm^3)
η_e	Effective porosity (cm^3/cm^3)
θ	Volumetric soil water content (cm^3/cm3)
$\theta (h)$	Soil moisture characteristic, also referred to as soil water retention curve
θ_r, θ_s	Residual, respectively saturated soil water content (cm^3/cm^3)
S_s	Specific storage or storativity (1/L, or m^{-1})
S_y	Specific yield (-, %)
v	Pore-water velocity, also referred to as tracer velocity (m/s)

Glossary

Term	Description
Adsorption	The binding of molecules to a particle surface. This process can bind methane and carbon dioxide, for example, to coal particles
Advection	The process whereby solutes are transported by the bulk mass of flowing fluid
Advection-dispersion equation (ADE)	Partial differential equation describing the total flux as the sum of the passive movement by advection and dispersion
Analytical model	A model that uses closed form solutions to the governing equations; here applicable to flow and transport processes
Aquifer	Rock or sediment in formation, group of formations or part of a formation, which is saturated and sufficiently permeable to transmit quantities of water to wells and springs
Aquitard	A saturated geological unit that is less permeable than an aquifer and incapable of transmitting useful quantities of water. Aquitards often form a confining layer over an artesian aquifer
Boundary condition	A mathematical expression of a state of a physical system that constrains the equations of the mathematical model. Boundary conditions can be at external and internal domain boundaries
Bounding estimate	A bounding estimate captures the highest possible exposure, or theoretical upper bound, for a given exposure pathway
Calibration	The process of refining the model representation of the hydrogeologic framework, hydraulic properties and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the groundwater flow system
Coal seam	Coal seams or coal deposits are sedimentary layers consisting primarily of coal. Coal seams can contain 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 to 97% pure methane, CH_4) typically extracted from permeable coal seams at depths of 300 to 1 000 m. Also called coal seam methane (CSM) or coalbed methane (CBM)
Coal seam gas produced water	Water that is pumped out of the coal seams to release the 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
Conceptual model	A conceptual model is a set of qualitative assumptions to describe a system, or part thereof. The assumptions would normally cover, as a minimum, the geometry and dimensionality of the system, initial and boundary conditions, time dependence, and the nature of the relevant physical, chemical and biological processes and phenomena
Confidence building	Confidence building in exposure assessment based on numerical modelling is achieved through adoption of a quality management system and associated quality assurance policy, and by demonstrating conceptual and

Term	Description
	numerical models are fit for purpose and used appropriately; such information must be provided in a transparent and traceable manner
Confined aquifer	An aquifer that is isolated from the atmosphere by an impermeable layer. Pressure in confined aquifers is generally greater than atmospheric pressure
Conservative approach / assessment	An assessment aimed at deliberately overestimating the potential risks to humans and the environment (after US EPA 1992)
Contaminant	Biological (e.g. bacterial and viral pathogens) and chemical introductions capable of producing an adverse response (effect) in a biological system, seriously injuring structure or function or causing death
Depressurisation	The lowering of static groundwater levels through the partial extraction of available groundwater, usually by means of pumping from one or several groundwater bores
Dewatering	The lowering of static groundwater levels through complete extraction of all readily available groundwater, usually by means of pumping from one or several groundwater bores
Dispersion or hydrodynamic dispersion	The spread of solutes, colloids, particulate matter, or heat by the combined processes of diffusion and physical mixing of fluids along the path of groundwater flow. This leads to a reduction of concentration at the macroscopic scale
Dispersivity	A geometric property of a porous medium which determines the dispersion characteristics of the medium by relating the components of pore velocity to the dispersion coefficient
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
Dual (or double) porosity	When two porosities may be associated with a hydrogeological system. An example is a porous rock with a fracture set; such a system may then have two characteristic porosities - one for the fractures (fracture or secondary porosity) and one for the porous matrix (matrix or primary porosity). Implied in this definition is that significant flow rates are present in both the fractures and the matrix
Effective porosity	The fraction of pores that are connected to each other and contribute to flow. Materials with low or no total porosity can become very permeable if a small number of highly connected fractures are present
Flowback water	The initial flow of water returned to a well after fracture stimulation and prior to production
Formation water	Naturally occurring water that is within or surrounding the coal, rock or other formations underground
Gaining stream	A stream that increases in discharge along its channel because of groundwater inflow
Geogenic chemical	A naturally-occurring chemical originating, for example, from geological formations.
Groundwater	Water occurring naturally below ground level (whether in an aquifer or other low permeability material), or water occurring at a place below ground that has been pumped, diverted or released to that place for storage there. This does not include water held in underground tanks, pipes or other works

Term	Description
Hazard	Inherent property of an agent or situation having the potential to cause adverse effects when an organism, system, or sub(population) is exposed to that agent
Heterogeneity	A characteristic of a medium in which material properties vary from point to point. For example, a sandstone may be more permeable in some layers than in others, and would therefore be described as heterogeneous. All aquifers are heterogeneous, although homogeneity is often assumed to simplify their analysis
High end estimates	A high end exposure estimate is a plausible estimate of the individual exposure for those persons at the upper end of an exposure distribution. Conceptually, the high end of the distribution means above the 90^{th} percentile of the population distribution, but not higher than the individual in the population who has the highest exposure
Hydraulic conductivity	A measure of the rate or velocity of groundwater flow through a material (such as soil / rock)
Hydraulic gradient	The change in hydraulic head between different locations within or between aquifers or other formations, as indicated by bores constructed in those formations
Hydraulic head	The potential energy contained within groundwater as a result of elevation and pressure. It is indicated by the level to which water will rise within a bore constructed at a particular location and depth. For an unconfined aquifer, it will be largely subject to the elevation of the watertable at that location. For a confined aquifer, it is a reflection of the pressure that the groundwater is subject to and will typically manifest in a bore as a water level above the top of the confined aquifer, and in some cases above ground level
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 hydraulic fracturing 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 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
Hydraulic properties	Properties of soil and rock that govern the transmission (e.g. hydraulic conductivity, transmissivity) and storage (e.g. specific storage, specific yield) of water
Hydrodynamic dispersion	The spreading (at the macroscopic level) of the solute front during transport resulting from both mechanical dispersion and molecular diffusion
Latin Hypercube Sampling (LHS) method	The LHS uses a stratified way of sampling from separate sampling distributions on the basis of a subdivision in intervals of equal probability, resulting in an efficient, and therefore, relatively small number of samples

Term	Description
Matrix (rock matrix)	The finer grained mass of rock material in which larger grains/crystals are embedded
Mechanical dispersion	A physical process that represents the mixing of solutes due to variations in flow velocities only. These variations are due to three primary factors: 1. variations in pore size 2. differences in path lengths 3. variations of velocities within each pore due to friction at the pore wall
Methane	The flammable gas (CH_4), which forms the largest component of natural gas
Molecular diffusion	A process at the molecular level that causes chemical movement in fluids and gases along a concentration gradient, from areas of higher concentrations to areas of lower concentrations
Monte Carlo (MC) analysis	Computational methodology to estimate the most probable outcome from a simulation model with uncertain inputs by generating multiple simulation runs from sampling input parameters from known probability distributions
Partial rank correlation coefficient (PRCC)	Measures the degree of linear relationship between input parameter X and output Y thereby removing the linear effect of all other remaining parameters
Permeability	The measure of the ability of a rock, soil or sediment to yield or transmit a fluid. The magnitude of permeability depends largely on the porosity and the interconnectivity of pores and spaces in the ground
Pore-water velocity	Also known as tracer velocity; is defined as the velocity of a non-adsorbing tracer in a porous media. It is calculated as $v = K \times i / n_e$, where K is the hydraulic conductivity, i the hydraulic gradient, and n_e the effective porosity
Porosity	The proportion of the volume of rock consisting of pores, usually expressed as a percentage of the total rock or soil mass
Probability density function	A mathematical description and depiction of the frequency distribution of a parameter
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
Produced water	Water that is pumped out of the coal seams to release the 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 back through the coal formation to the well along with the gas, and is pumped out via the wellhead
Recharge	Groundwater recharge is the process whereby surface water (such as from rainfall runoff) percolates through the ground to the watertable
Risk	The probability of an adverse effect in an organism, system, or (sub)population caused under specified circumstances by exposure to an agent
Risk assessment	A process intended to calculate or estimate the risk to a given target organism, system, or (sub)population. This includes 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

Term	Description
	characteristics of the specific target organism
Risk quotient	Risk quotients are calculated by dividing exposure estimates (i.e. predicted environmental concentrations or PECs) by the acute and chronic ecotoxicity values (i.e., RQ = PEC/Toxicity value)
Saturated flow	Flow through a porous medium (such as soil or rock) in which the void space within the porous medium is entirely occupied by water (as opposed to water and gas)
Saturated zone	That part of Earth's crust beneath the regional watertable in which all voids, large and small, are filled with water under pressure greater than atmospheric
Sediment	A naturally occurring material that is broken down by processes of weathering and erosion, and is subsequently transported by the action of wind, water or ice, and / or by the force of gravity acting on the particle itself
Shallow groundwater	Groundwater that occurs in the shallowest aquifer, bounded by a watertable and an unsaturated zone of variable thickness (sometimes absent) above, and by deeper aquifer or aquitard systems below. Also generally referred to as the watertable aquifer
Solute	Material dissolved in a liquid (or solvent)
Stochastic model	A model where both inputs and output can be represented by probability distribution functions
Stygofauna	Animals that inhabit groundwater, either entirely or substantially. Most are invertebrate crustaceans, but the term also encompasses snails, mites, underground beetles and some fish
Surface impoundment	A natural topographic depression, artificial excavation, or dyke arrangement for storing clean water, pure fracturing fluids, or wastewater. A surface impoundment may be constructed above the ground, below the ground, or partly above the ground and partly below the ground. A surface impoundment’s length or width is greater than its depth (e.g. it is not an injection well)
Tortuosity	The non-straight nature of soil or aquifer pores
Toxicity	Inherent property of an agent to cause an adverse biological effect
Transparency	Transparency is an attribute of a report that is: ‘…written in such a way that its readers can gain a clear picture, to their satisfaction, of what has been done, what the results are, and why the results are as they are…’.
Traceability	Traceability is an unambiguous and complete record of the decisions and assumptions made, and of the models and data used in arriving at a given set of results
Unconfined aquifer	An aquifer in which there are no confining beds or layers between the saturated zone and the ground surface, so the watertable can fluctuate as a moving upper boundary at the top of the saturated zone
Unconventional gas	Natural gas found in a very low permeability rock, such as shale gas and coal seam gas
Unsaturated flow	Flow through a porous medium (such as soil or rock) in which the void space within the porous medium is occupied by both water and gas (rather than water only)

Term	Description
Upper bound estimate	A bounding estimate that captures the highest possible exposure, or theoretical upper bound, for a given exposure pathway
Vadose zone	The vadose zone, also called the unsaturated zone, extends from the top of the ground surface to the watertable. In the vadose zone, the water in the soil pores has a pressure less than atmospheric
Water balance	A process of equating the water inflows to a groundwater system with the water outflows, accounting for any changes in storage of water in the system
Watertable	The surface between the unsaturated zone and the saturated zone. The groundwatertable can also be defined as the surface at which groundwater pressure is equal to atmospheric pressure

Contents

Tables

Figures

1 Introduction

1.1 Purpose of this report

This report documents the conceptual modelling framework to predict environmental concentrations of hydraulic fracturing fluids in spills and leaks at the land surface, and their anticipated fate pathways: soil; shallow groundwater; wetlands and streams. This forms the basis for determining human exposure to hydraulic fracturing chemicals present at the land surface.

The term shallow groundwater is used here to represent all groundwater in unconfined aquifers typically up to several tens of metres deep that is hypothesised to be receiving contaminants released from the land surface. These are mainly the alluvial aquifers and weathered rock aquifers adjacent to the alluvial aquifers; they are bounded by a watertable and an unsaturated zone of variable thickness (sometimes absent) above, and by deeper aquifer or aquitard systems below.

Exposure assessment for deep groundwater is not within the scope of the current project. Deep groundwater refers mainly to confined aquifers, typically several hundreds of metres below ground surface, that would not normally be affected by surface-derived contamination, or to the deeper parts of unconfined aquifers in contact with coal formations targeted for gas extraction (e.g. through active faults or permeable formations between coal and overlying aquifers, or via a defective coal seam gas well into the overlying aquifer). Future research could quantify fate pathways of drilling and hydraulic fracturing fluids within a coal seam gas well field and its surrounding deep groundwater.

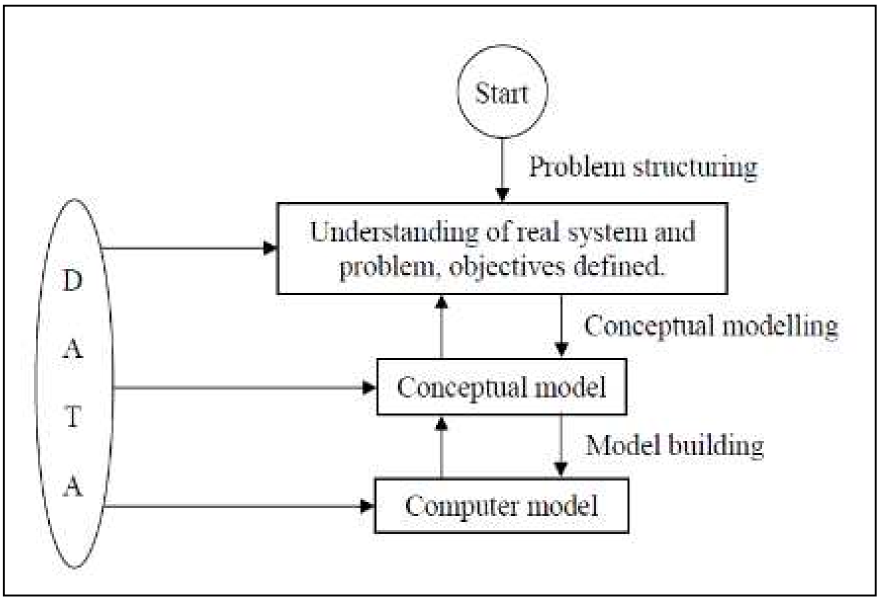
The conceptualisation process considered pathways of chemical transport through soil and shallow groundwater, with soil pore water and shallow drinking water wells as receiving environments. Wetlands and streams were also considered as receiving environments for the downstream discharge of shallow groundwater at the surface. Chemical concentrations calculated in these receiving environments provided input to the exposure assessment calculations for human receptors. For the purpose of calculating chemical concentrations in receiving environments, conceptual flow and transport models for soil (or the unsaturated zone) and shallow groundwater (the saturated zone) were developed. To allow an integrated exposure assessment to be completed, a parallel conceptualisation and modelling process was developed for calculating chemical concentrations in the receiving surface water environments.

1.2 Approach

A step-wise approach to investigating risks associated with coal seam gas extraction (i.e. addressing shallow groundwater first and deep groundwater later) is justified because it allows prioritisation of research efforts where the anticipated risks are highest, and it allows for preparatory studies to take place in regards to fracture growth and the spreading of chemicals in the coal seam gas well field and its surrounding sediments and deeper aquifers (Jeffrey et al. 2017b, 2017c). Recent reviews in the US and Europe have shown that the greatest risks associated with unconventional gas exploitation are associated with the accidental release or spill of hydraulic fracturing fluids associated with surface operations, resulting in contamination of soil, shallow groundwater and surface water (Lechtenböhmer et al. 2011; The Royal Society and The Royal Academy of Engineering 2012). In a recent literature review Mallants et al. (2017a) reported that between the years 2009 and 2013, the majority of compliance-related incidents involving gas extraction were spills involving the release of coal seam gas water (i.e. flowback and / or produced water) during operations (59%).

The conceptual modelling framework developed in this study thus has a focus on capturing the key features of a source-pathway-receptor system that describes the impact of spills and leaks from drilling and hydraulic fracturing fluids, including flowback and produced water, on soil and shallow groundwater. This involves developing a conceptual soil and groundwater model, where the model is a descriptive representation of a soil-groundwater system that incorporates an interpretation of the geological and hydrological conditions (Anderson and Woessner 1992). It consolidates the current understanding of the key processes of the soil-groundwater system, including the influence of stressors, and assists in the understanding the effects of possible future changes.

Conceptual modelling is the stage in the simulation process that determines the appropriate spatial scale and level of process detail to model. The relationship between the conceptual modelling stage and other project tasks that come at the beginning of a simulation project (such as, for example, problem formulation, or model building) are illustrated in Figure 1.1 (Brooks 2007). The conceptual modelling stage specifies how reality will be simplified in terms of process representation, variability of key properties, stressors and equations that describe the processes (Barnett et al. 2012; Brooks 2007). Moreover, the conceptual modelling stage includes specifying the type of model (e.g. transient or steady-state; discrete or continuous changes of state), the scope (the question that the model is expected to address) and the geometric boundary of the model (Brooks 2007). Figure 1.1 shows that the modelling process is generally not linear but iterative; for example, conceptual modelling and model building typically takes place in such an iterative manner to allow for improvements of the conceptual model based on insights obtained from computer simulation results (e.g. sensitivity analysis). Conceptual modelling is generally a non software-specific description of the computer simulation model being developed (Robinson 2008).



Source: Brooks (2007)

Figure 1.1 Outline of the initial tasks and outcomes in a simulation project. Other tasks that follow include verification and validation of the model and output analysis

The aim of conceptual modelling is to choose the model that will give the best overall project performance (Brooks 2007). There are different aspects of performance that need to be considered (for example, results, future use of the model, confidence in the model, resources required). Brooks and Tobias (1996) elaborate on these aspects as summarised in Table 1.1

For each of the above elements, minimum performance standards should be identified that will lead to the most successful outcome for the project as a whole (Brooks and Tobias 1996).

In line with the approach for identifying drilling and hydraulic fracturing chemicals of low human health concern [based on the Inventory Multi-Tiered Assessment and Prioritisation (IMAP) Framework developed by NICNAS] the first tier of a multi-tiered approach was developed for the soil and groundwater pathway. At the lowest level or tier (i.e. Tier 1), solute transport in soil and groundwater neglect chemical interactions between contaminants and the solid phases (minerals and organic matter) and biogeochemical transformation. A Tier 1 assessment uses generic, high end estimates of the range of site properties influencing chemical transport such that the assessment results have the broadest applicability (i.e. not site specific). The advantage of this approach was that if the result of the Tier 1 assessment demonstrated compliance with the relevant criteria for protection of human health and the environment, there is a higher level of confidence that under real conditions the impact would be considerably less. This follows from the consideration that in reality, chemical attenuation is likely to play a much more prominent role and distances between source and receiving environments will be much longer than those considered for producing high end estimates. The approach adopted is therefore conservative and may overestimate chemical concentrations.

Table 1.1 Criteria for evaluating simulation project performance

Issue	Criteria for evaluating simulation project performance
Results	• The extent to which the model output describes the behaviour of interest (whether it has adequate scope and detail) • The accuracy of the modelling results • The ease with which the model and its results can be understood. • Future use of the model • The portability of the model and the ease with which parts of the model can be reused in future models.
Confidence in the model (for a detailed discussion, see Section 6)	• The probability of the model containing errors • The accuracy with which the model output fits the historical data • The strength of the theoretical basis of the model including the quality of the input data. • Degree to which model sensitivity has been tested • Degree to which uncertainty has been identified, quantified, and reduced.
Resources required	• The time and cost to build the model, including data collection, verification and validation • The time and cost to run the model • The time and cost to analyse the results of the model • The hardware requirements of running the model • The cost of acquiring the software and of maintaining an annual licence.

The conceptual model for the unsaturated zone accounts for different solute sources at the land surface and their characteristics. The fate pathways, for which detailed conceptual models have been developed here, included spills from small containers (a few litres) to large totes (several thousands of litres), and short-term and long-term leakage from untreated water storage ponds (containing flowback and / or produced water) under conditions of normal operation. Applying the advection-dispersion equation for an imposed small water flux equal to the assumed leak rate followed by an average groundwater recharge rate representative of soil conditions after dismantling of the storage ponds meant that solute transport across the soil profile could be simulated. The use of different thicknesses for the unsaturated zone accounted for the observed variability in depth from land surface to the watertable. The model for the unsaturated zone allows calculation of environmental concentrations and subsequent derivation of dilution factors at the interface of the unsaturated zone with the groundwatertable.

The usefulness of a Tier 1 assessment with a generic groundwater model is limited when the results need to be representative of a broad set of hydrogeological conditions. In the context of the National Coal Seam Gas Chemicals Assessment, such a broad set of hydrogeological conditions is informed by the priority bioregions agreed by the Australian Government. Rather than developing several region-specific groundwater models, a complex undertaking that is not necessary in a Tier 1 approach aimed at delivering high end estimates, a limited set of groundwater flow models in a single sub-bioregion were developed. These models were then used as a basis for more detailed groundwater transport calculations to derive precautionary, high end predictions of environmental concentrations. This regionalised generic approach used a single conceptual model with a broad range of parameter values. This kind of approach also allows a high throughput evaluation of chemicals (i.e. efficient analysis of a large number of chemicals) while still considering a broad range of hydrogeological conditions.

A three-dimensional regional-scale groundwater flow model previously developed for the Namoi Catchment Water (NCW) Study (SWS 2012a) was used as the basis for developing a small-scale conceptual model for chemical exposure assessment of the groundwater flow pathway. As the NCW Study is relatively recent, well documented, and has a rigorously tested alluvial aquifer model component with very good (demonstrated) performance, it was selected as the one to be adapted and used for the purposes of evaluating environmental concentrations of chemicals associated with spills and leaks.

From the regional Namoi Catchment Groundwater Model, two areas were initially identified for which sub-regional (called "local" in these reports) groundwater flow models could be developed into a tractable area for more detailed modelling that incorporated all of the relevant features that were needed. On the basis of several criteria, one out of those two areas was then selected for developing a groundwater flow model. The initial selection of the two areas was based on consideration of:

- potential for future risk based on ongoing and planned activities with regards to coal seam gas extraction
- sufficiently representative in terms of broad coverage of hydrogeological features
- sufficiently representative in terms of receiving environments of relevance to both human and environmental receptors.

The final selection of a single area for developing the local model resulted in an area located near Narrabri, within the Upper Namoi model. The area contains a major stream (the Namoi River) with a considerable gaining stream segment. The area also contains the Gunnedah Formation (up to 115 m in thickness), which consists predominantly of gravel and sand with minor clay beds and is the principal aquifer used for irrigation in the region. It also contains several relevant receiving environments including shallow groundwater and shallow water wells in the alluvial aquifer, and groundwater dependent wetlands.

Uncertainties associated with the soil and groundwater flow and transport models mainly relate to uncertainties about model parameters used and uncertainties about the conceptual model that was initially developed. A first step to address uncertainties associated with the model parameters was undertaken by identifying a range of plausible parameter values based on the Namoi Catchment Groundwater Model. After exposure calculations were undertaken, soil and groundwater models were run multiple times using those different parameter values to quantify propagation of parameter uncertainty through the model to determine how differing values affect model output. Uncertainties in the conceptual model were addressed by developing simplified conceptual models based on high end estimates of parameters that are not likely to underestimate impact. Accounting for the effects of uncertainty analyses will also help to bracket the range of solute concentrations that key receptors may be exposed to.

A comprehensive approach to ensuring confidence in the numerical modelling process and the reporting of its outputs is also presented. Elements of confidence building in the mainstream of quantitative impact assessments included:

- rigorous record keeping and quality assurance procedures to ensure the calculations and results are those intended, and are fully traceable and reproducible
- scientific and technical understanding of the processes and events involved, i.e. justification of the information that is compiled in the assessment basis
- models, codes and data that are ensured through the verification, qualification and, when possible, validation process
- a system of completeness checks to ensure that all relevant processes and events are represented and treated appropriately in the impact assessment
- uncertainty management that ensures relevant uncertainties are considered and either treated or their effects acknowledged.

Drawing on the information analysed during the previously conducted reviews of the available literature (DoEE 2017a; Jeffrey et al. 2017a; Apte et al. 2017; Mallants et al. 2017a), and the report on the identification of chemicals associated with coal seam gas extraction in Australia (NICNAS 2017c), there is a high degree of confidence in the conceptualisation of the pathways to estimate exposure concentrations. As a result, the near-surface groundwater transport pathway for chemicals can be utilised directly to inform the human health risk assessment processes being conducted by the National Coal Seam Gas Chemicals Assessment.

2 Background and context

2.1 Background

The conceptualisation stage of this project included development of conceptual exposure pathway models and a set of risk simulator modelling tools for estimation of release, consideration of environmental fate, and derivation of predicted environmental concentrations (PEC) in soil and shallow groundwater from surface handling, such as site spills, overflows, runoff, and leaks from surface ponds (Mallants et al. 2017b). Using such modelling tools, concentrations, distributions and travel times for environmental contaminants will be determined for specific exposure scenarios and modelling assumptions identified as reflective of particular geographic regions in which gas extraction operations are being conducted (see Mallants et al. 2017b).

This report builds on the previous literature reviews (Jeffrey et al. 2017a; Apte et al. 2017; Mallants et al. 2017a; DoEE 2017a; NICNAS 2017a) and provides key input into the calculation of environmental concentrations in shallow groundwater from surface spills and leaking ponds. Predicted environmental concentrations were then used to calculate the risk to workers and the public (by NICNAS).

2.1.1 A tiered approach

The National Coal Seam Gas Chemicals Assessment framework includes predicting environmental concentrations in soil, shallow groundwater and surface water. In line with the approach for identifying drilling and hydraulic fracturing chemicals of low human health concern, based on the Inventory Multi-Tiered Assessment and Prioritisation (IMAP) Framework developed by NICNAS (NICNAS 2014), the first tier of a multi-tiered approach was developed for the soil and groundwater pathway. At the lowest level or tier (i.e. Tier 1), solute transport calculations in soil and groundwater are without chemical interactions between contaminants and the solid phases (minerals and organic matter), and without biogeochemical transformation. Also, short distances between source and receiving environment are deliberately used to overestimate impact. A Tier 1 assessment used generic site properties such that the assessment results have broad applicability and produce high end estimates that tend towards protecting public and environmental health by not underestimating risk in the face of uncertainty and variability. Higher tier assessments will produce more realistic impacts because they include processes that would result in a higher degree of attenuation by considering adsorption to minerals and organic matter to take place and by considering biodegradation of organic chemicals (Tier 2), and the subsurface characteristics would also be more site-specific (Tier 3). Higher tiers would be required only when it cannot be demonstrated at the first tier that the impact is not exceeding the regulatory criteria. Such an approach is consistent with the tiered approach to exposure assessment developed by the US Environmental Protection Agency (US EPA) (2004a) and by the Australian Environment Protection and Protection Council's environmental risk assessment guidance manulas (EPHC 2009a and 2009b) (Figure 2.1). Note that the number of tiers used in any assessment is at the discretion of the assessor based on objectives, local conditions, data availability, etc. There can thus be several variants of the generic multi-tiered methodology described in Figure 2.1.

For the human exposure assessment involving leakage to shallow groundwater a Tier 1 approach has been adopted. This is based on consideration of:

- a simplified leakage model for the soil pathway (see Section 5.2)

- groundwater flow and chemical transport model for the groundwater pathway (see Section 5.3).

These considerations would result in deliberately overestimating exposure. Although site-specific data was used where available, its spatial resolution, or "granularity", is limited and only data relevant to flow characteristics but not biogeochemical properties was used. The environment risk assessment was a three-tier process but did not draw on the shallow groundwater modelling (DoEE 2017c).

The advantage of an assessment based on high end parameter estimates is that if the result of the assessment demonstrates compliance with regulatory criteria, one can be reasonably confident that under real conditions, when attenuation of chemicals is likely to play a much more prominent role, the impact will be considerably less. We note however that attenuation may decrease with time for large amounts of contaminants that leak into groundwater, thus causing saturation of sorption sites.

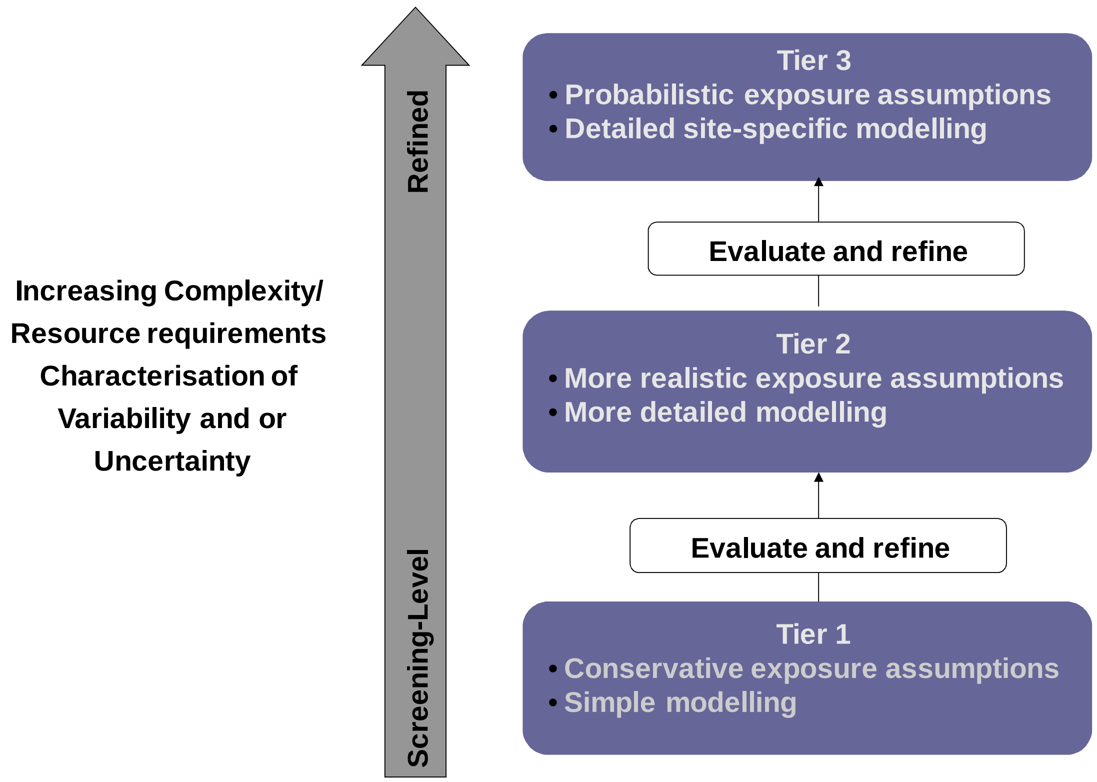
Exposure assessments for humans (carried out by NICNAS) require predicted environmental concentrations (PECs) in relevant receiving environments such as soil, shallow groundwater and surface waters (rivers, wetlands, springs) that receive groundwater through discharge processes. To generate PECs CSIRO developed models that calculate:

- chemical concentrations in such receiving environments
- spatial distribution of chemicals in groundwater
- spatial probability or likelihood of occurrence of receptors
- travel time through soil from the surface source to the groundwatertable
- travel time from (groundwater) source to receptors (such as groundwater wells and discharge zones in river alluvium) assuming realistic but high end estimates, scenarios, and modelling assumptions.

The results of exposure assessments (i.e. the PECs for soil, groundwater, wetlands and rivers) may be integrated with ecotoxicity data to calculate the risk quotient (RQ). Risk quotients are calculated by dividing exposure estimates (i.e. PECs) by the predicted no effect concentration (PNEC), i.e., RQ = PEC/PNEC. For example, for any given chemical, its RQ value allows a risk classification in accordance with the principle outlined by EPHC (2009) and ARMCANZ and ANZECC (2000) guidelines:

- Chemicals with RQ < 1: chemicals of 'low concern'; unlikely to have adverse environmental impacts if used in accordance with the assessment scenarios
- Chemicals with RQ ≥ 1 and < 10: chemicals of 'potential concern'; further risk mitigation measures may be required if the chemical is used
- Chemicals with RQ ≥ 10: chemicals of 'potentially high concern'; further risk mitigation measures are likely to be required if the chemical is used.

Tier 1 assessments are typically generic and based on high end estimates. Consequently, there is less of a need for a highly accurate and detailed model representation of site-specific subsurface processes and properties. For instance, while appropriate modelling of the surface water to groundwater interactions is important for quantifying groundwater and solute fluxes into gaining streams, developing detailed site-specific models of surface water to groundwater interaction is beyond the scope of the current project. The exposure assessment will provide chemical concentrations in surface water as a result of groundwater discharge processes. Different model assumptions will be considered in the assessment. For instance, consequences can be shown to be significant if the contaminant source is within a given distance from the river. If such circumstances have a sufficiently high likelihood to occur in reality, future studies will need to consider improving the interaction between groundwater and surface water in models (this could be at the Tier 3 level for a detailed site-specific analysis).



Adapted from US EPA (2004a)

Figure 2.1 Example of tiered approach to exposure assessment

2.1.2 A conservative approach

More often than not, there is insufficient knowledge about the behaviour of chemicals in soil and groundwater following spills and leaks. The lack of knowledge is due to measurement uncertainty, variability in the available data, and data that has not been determined previously. As a result, risk cannot be known or calculated with absolute certainty (US EPA 2004c). To address these uncertainties, regulators and environmental protection agencies have developed risk assessment procedures that tend towards protecting public and environmental health by preferring an approach that does not underestimate risk in the face of uncertainty and variability (US EPA 2004c). In other words, they seek to adequately protect public and environmental health by ensuring that risk is not likely to be underestimated. This is generally achieved through the use of some high end estimates of the various parameters informing the risk assessment process.

In this regard US EPA (1992) distinguishes bounding estimates and high end estimates. A bounding estimate captures the highest possible exposure, or theoretical upper bound, for a given exposure pathway. Exposure scenarios (‘bounding’ scenarios) for derivation of bounding estimates combine assumptions that results in a highly conservative exposure estimate. A high end estimate means at the high end of the distribution, or above the 90th percentile of the population distribution, but not higher than the individual in the population who has the highest exposure.

High end estimates of exposure (i.e. in the top 10% of the real distribution) are generally considered to be more realistic or more likely to occur compared with bounding estimates (i.e. the highest exposure to date). Such estimates are derived from scenarios ('realistic bounding' scenarios) with more realistic assumptions. This realistic-precautionary approach still seeks not to underestimate risk, and uses realistic but still precautionary assumptions and parameter values where available. The current exposure assessment uses realistic bounding scenarios to produce high end estimates of exposure.

A risk analysis then combines the likelihood of occurrence of events with the severity of consequence of those events to characterise the level of risk, often using a risk rating matrix (see, for example, Figure 2.2). The risk rating matrix may be qualitative, semi-quantitative or quantitative depending on the degree of confidence in specifying events and their likelihood. The likelihood associated with a certain consequence (e.g. receptor responses based on concentrations in receiving environments) can be quantified through analysis of the results of multiple model runs. These results can be used to produce probabilities of exceeding certain consequences. Such results can help quantify uncertainty in model results and data.

Severity of consequence

			1	2	3	4	5
		Descriptor	Insignificant	Minor	Moderate	Major	Catastrophic
Likelihood level	A	Almost certain	A1	A2	A3	A4	A5
	B	Likely	B1	B2	B3	B4	B5
	C	Possible	C1	C2	C3	C4	C5
	D	Unlikely	D1	D2	D3	D4	D5
	E	Rare	E1	E2	E3	E4	E5

Level of risk

Low	Moderate	High	Extreme

Adapted from DRET (2008). This is the minimal and simplest form of a risk rating matrix and is useful where consequences and likelihoods can be defined in qualitative terms.

Figure 2.2 An example of a qualitative risk rating matrix where consequence ratings range from 'insignificant' (1) to 'catastrophic' (5) and likelihoods range from 'rare' (E) to 'almost certain' (A)

Benefits of a risk analysis include:

1. exploring the issues of impact, likelihood and risk within a scientific and logical framework
2. providing insights into where high value water assets (for example water dependent listed threatened species and state listed important water features) may face high risks
3. identifying where risks may occur that have previously not been identified or have been underestimated.

2.1.3 Selection of model study area and receiving environments

This report describes conceptual soil and groundwater models for water flow and solute transport modelling, with a focus on shallow groundwater and interactions with receiving surface waters, initially within the Namoi catchment in northern NSW (Figure 2.3). The Namoi catchment was selected for the purpose of demonstrating the exposure assessment framework associated with leakage of hydraulic fracturing fluids from surface sources for the following reasons:

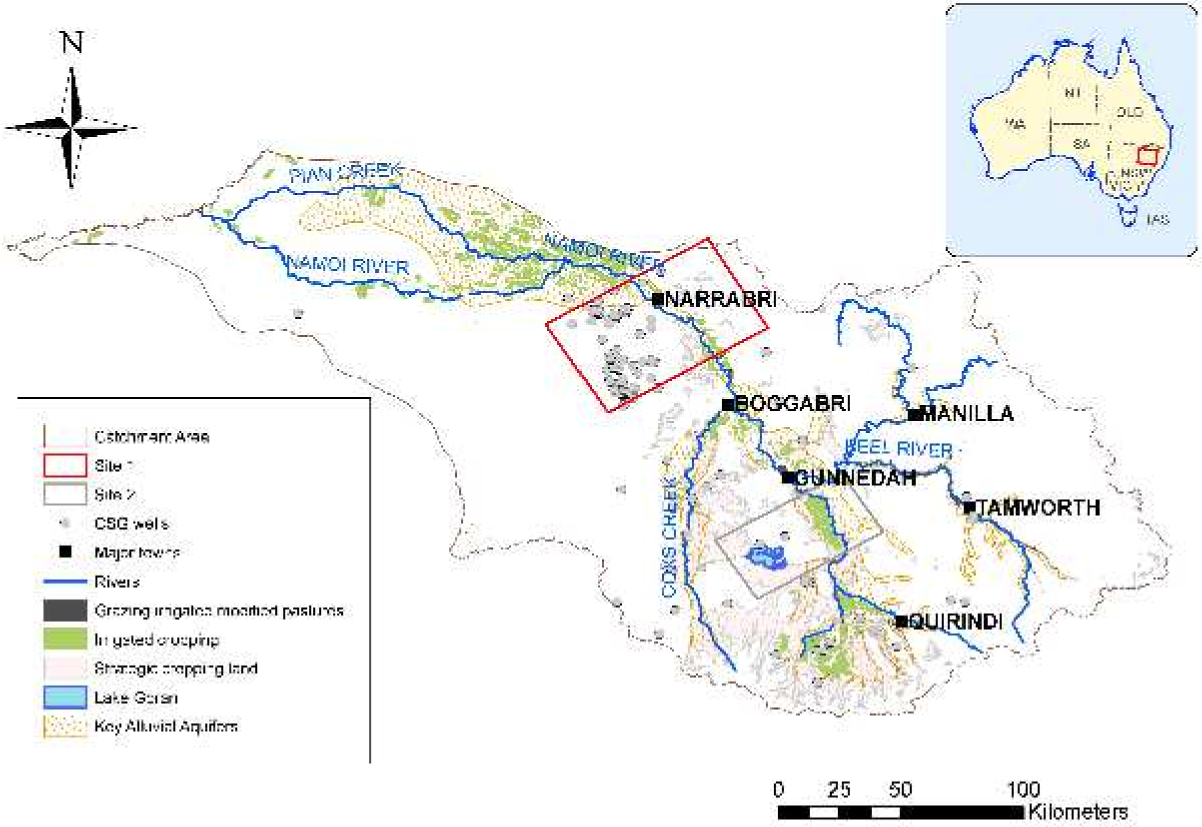
- the key relevant receiving environments, as identified in DoEE (2017a), are present in a relatively small area facilitating the use of a limited number of models to represent a broad range of receiving environments
- coal seam gas extraction is being trialled and is expected to be developed across a relatively large area which includes important receiving environments for humans and the environment
- existing groundwater flow models could be relatively easily adapted and made fit for purpose within the short timeframe of this project

An assessment of the limitations of such existing groundwater models for their intended use in this project was made (see Section 4.2). It is important to recognise that model limitations are linked to their intended use, and that limitations for one application do not automatically mean the model has limitations for all other applications. These issues, and associated limitations, are examined in detail in Section 4.2.

For the purposes of this exposure assessment, the most important receiving environments connected to soil, shallow groundwater, wetland and streams are (refer to Figure 2.3):

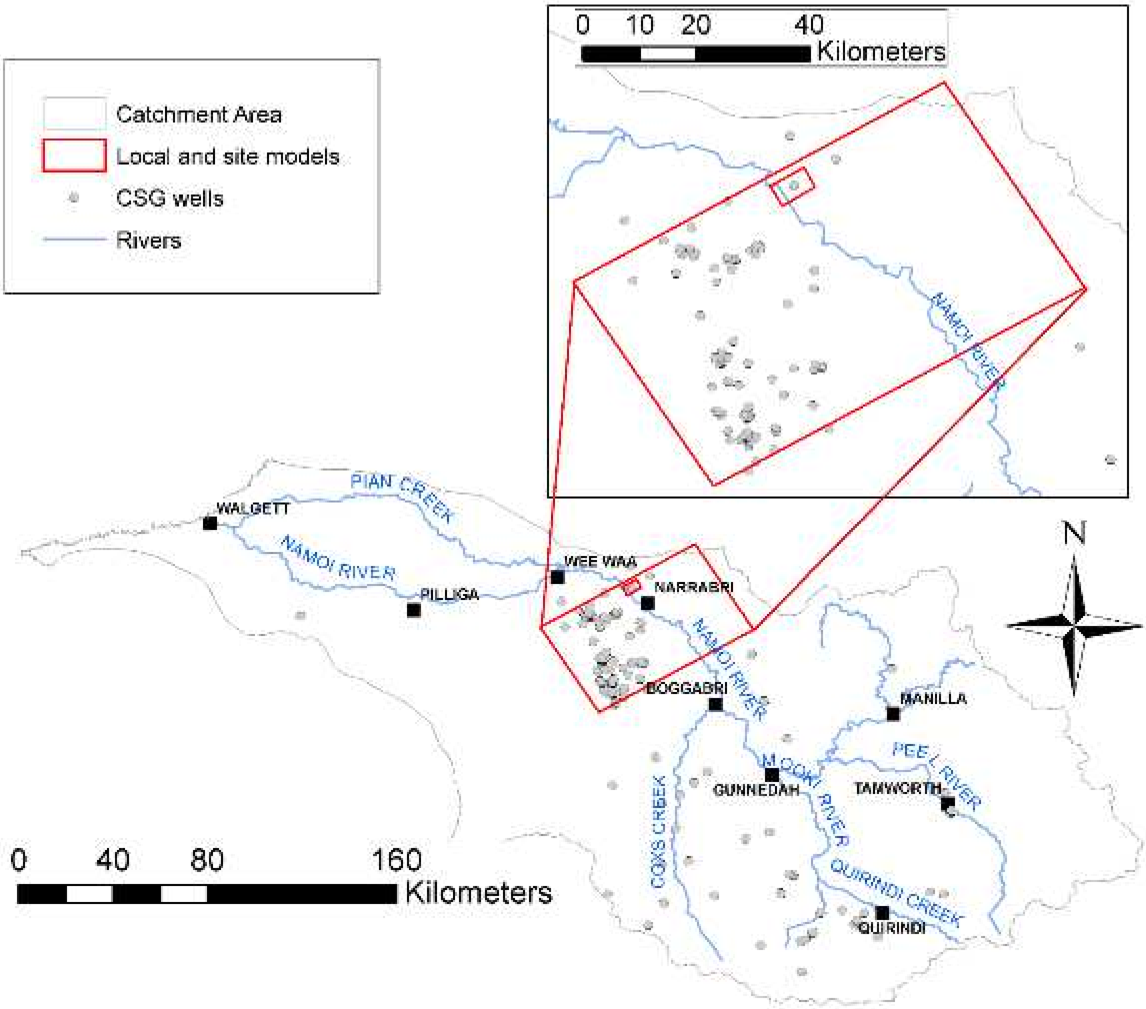
- soil itself as the primary receiving environment of unintentional spills at a coal seam gas site (see Section 5.2). The intentional release of associated water (treated or untreated) occurs in the case of irrigation of agricultural land or for dust suppression on roads or coal seam gas sites (for derivation of PECs associated with irrigation and dust suppression the reader is referred to DoEE 2017c)
- shallow groundwater systems with considerable groundwater use for drinking water, irrigation and stock, and recreation (a detailed discussion is provided in Section 5.3.2.3)
- important hydrological features (for example, the Namoi River, numerous wetlands and swamps) (a detailed discussion is provided in Section 5.3.2.4)
- important (or iconic) environmental assets (including threatened freshwater flora and fauna species) (a detailed discussion is provided in Section 5.3.2.4).

Coal seam gas activities (mainly exploration with some wells in production) within the Namoi catchment in NSW's Gunnedah Basin began in 2008. Figure 2.4 shows the location of coal seam gas wells, including those that produce gas, those that do not produce gas and those that are permanently sealed. Note that while the location of these wells is used in this study, the study is not an assessment of the risks associated with these wells or the risks associated with any specific coal seam gas extraction project.



Source: NSW Government (2014a); NSW Spatial Data Catalogue (accessed: 2014 via https://sdi.nsw.gov.au/catalog/main/) and Geoscience Australia (accessed: 2014 via http://www.ga.gov.au/metadata-gateway/metadata/record/76313/).

Figure 2.3 Namoi catchment with indication of subregions selected for model testing (rectangles labelled Sites 1 and 2). Also shown are coal seam gas wells and receiving environments (alluvial aquifers, agriculture, and wetlands)



Source: NSW Spatial Data Catalogue (accessed: 2014 via https://sdi.nsw.gov.au/catalog/main/) and Geoscience Australia (accessed: 2014 via http://www.ga.gov.au/metadata-gateway/metadata/record/76313/). Coal seam gas wells shown include wells that produce gas, wells that do not produce gas, and well that are permanently sealed (see www.csg.nsw.gov.au).

Figure 2.4 Coal seam gas wells in the Namoi catchment of the Gunnedah Basin

Several groundwater models exist for the Namoi catchment. Because the main objective of the current exposure assessment is to quantify fate pathways involving shallow groundwater, the Namoi Catchment Model [SWS 2010, 2011, 2012a, 2012b]) commissioned by the NSW Government in August 2010 as part of the Namoi Catchment Water Study was chosen as the basis for our exposure assessments.

2.1.4 Extrapolation to other areas

For the purposes of exposure assessments in this study, the consideration of the receiving environment only includes the six priority areas for bioregional assessment. To demonstrate the feasibility of an exposure assessment framework that includes predicting environmental concentrations of contaminants in soil and shallow groundwater, a generic, regionalised approach was used as it allows a high throughput evaluation of a large number of drilling and hydraulic fracturing chemicals. Developing several region-specific groundwater models is not feasible within the available timeframe and resources. Highly detailed, region-specific exposure assessments would also be excessive for high end estimates and Tier 1 chemical risk assessments. The approach used in this exposure assessment was to utilise existing peer reviewed ‘off the shelf’ models to develop a limited set of groundwater flow models in a single catchment. Such sub-domain simulators represent several typical hydrogeological conditions which allow model results to be sufficiently generic while remaining highly efficient in terms of chemical throughput. These models form the basis for detailed precautionary groundwater transport calculations.

For results from the regionalised generic approach to be applicable to other coal seam gas areas (bioregions), several calculation cases will be defined within the same model domain by perturbing key flow and transport parameters within physically realistic ranges. Model parameters relevant for groundwater flow and transport include hydraulic conductivity (*K*), hydraulic gradient (*i*) and effective porosity (n_e) (these three parameters together define the pore-water velocity:

$$V = K \times \frac{i}{n_e} \qquad \text{[Equation 1]}$$

Where:

K = hydraulic conductivity

I = hydraulic gradient

n_e =

Variations were also considered for soil parameters (soil thickness, recharge and leakage rate, depth-dependent hydrodynamic dispersion) and distance to receiving environments for the groundwater pathway. The exposure assessment should be able to explore a sufficient range of hydrogeological conditions and materials (e.g. alluvial gravel, alluvial sand, coastal sand, sandstone, fractured rock) to demonstrate that the exposure assessment framework is fit for purpose. The range of each of these parameter values will be determined by the natural variability observed in an area that is larger than the simulation domain. By running the regionalised generic model this way, multiple results based on varying ranges of key parameters can be generated. In doing so, the results become applicable to a larger area than the domain used in the calculations. A demonstration of the degree to which extrapolation to other areas may be achieved is available from Mallants et al. (2017b).

Transferability to other regions for which no detailed solute transport calculations exist, or for which no groundwater models exist, is possible provided the hydrogeological conditions can be quantified in broad classes of groundwater velocity and travel times from source to receiving environment. Expert knowledge can be used to develop such classes and compare them with the conditions of the detailed exposure assessments. Although this is a generic and semi-quantitative to qualitative approach, it is a defensible way for a screening level analysis. Biogeochemical processes that contribute to natural attenuation (e.g. sorption, precipitation, (micro)biological degradation and radioactive decay) are not considered at this stage. However, the simplified models can easily be expanded to include such processes if the risk assessment for humans and / or the environment indicates non-negligible consequences based on high end estimates and assumptions. Typical numerical models for this purpose include MODFLOW for groundwater flow and MT3D for chemical transport (Mallants et al. 2017a).

2.1.5 Numerical model selection

This exposure assessment included development of a three-dimensional numerical model to predict the potential impacts of a number of different mining and gas developments on existing water resources. The Namoi Catchment Model (NCM) produced by Schlumberger

Water Services (SWS) is a recent and well-documented model of which the alluvial model components, representing the shallow aquifers along river channels, had been rigorously tested. It is understood that the NCM was originally developed for predicting the effect that the extraction of groundwater associated with coal seam gas operations may have on the regional groundwater system. This means that the focus was on modelling deep groundwater and its response to coal seam gas-related water extraction and how depressurisation in deep groundwater would affect the very shallow groundwater. A summary of the conceptual underpinnings of the NCM is provided in Section 4, together with a summary of arguments why some components of this model are fit for purpose. This will serve as a starting point for developing more detailed flow and transport models.

Two areas within the Namoi Catchment Model were preselected for testing their suitability for detailed flow and transport calculations. Due to time and resource limitations, only one of the two areas will be used for detailed calculations. For reliable solute transport calculations, the numerical grid has to be sufficiently small to reduce numerical dispersion and oscillations (Konikow 2011), to allow proper representation of large concentration differences over short distances, and to allow proper representation of solute sources and receiving environments. Konikow (2011) demonstrates a greater lateral spreading of the solute plume when the solute transport models changed from a 2 m grid spacing to a 50 m grid spacing. Therefore, as a basis for the conceptual groundwater model, the current exposure assessments utilises smaller domains (at most a few km^2) with refined numerical grids for which the computational requirements are not excessive. Area 1 is located to the south of the Namoi River and the town of Narrabri, while Area 2 is located around Lake Goran (Figure 2.3). These two areas have a sufficient representation of key receiving environments in coal seam gas development areas. A more detailed assessment of their suitability for solute transport calculations is considered in Section 5.3.3.

While only one out of the two areas will be selected for detailed and realistic flow and transport calculations, multiple model runs will be made with a regionalised generic sub-domain model developed for hypothetical leaks and spills involving hydraulic fracturing fluids due to coal seam gas extraction activities. The regionalised generic model runs will be based on a specific site, with hypothetical but realistic exposure scenarios identified as reflective of particular geographic regions in which coal seam gas extraction activities are being conducted. This approach considers one conceptual model for exposure assessment, but the model will be run with different parameter values. In other words, the geometry of the model domain and the architecture of the geological formations will not change; only model parameters will be updated.

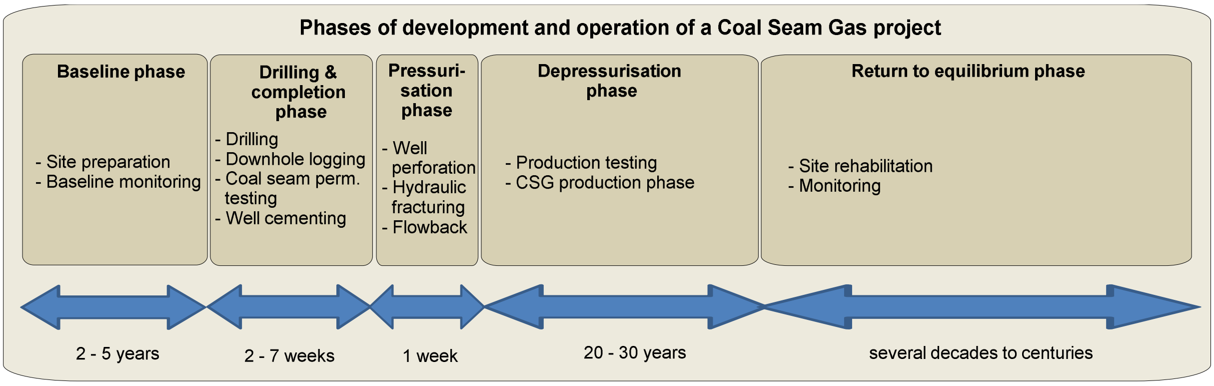
In addition to groundwater models, the exposure assessment will also need to develop and apply a soil water balance and solute transport model for the purpose of calculating the solute flux at the soil / groundwatertable interface (as the soil is part of the soil-to-groundwater solute pathway); and calculating the solute concentration in the soil profile in case the (vegetated) soil is a receiving environment. Conceptual soil models and leaching scenarios are discussed in Section 5.2. Unlike for groundwater flow modelling, no fit for purpose solute transport models for the unsaturated zone are currently available for the Namoi catchment. Therefore, very simplified models will be developed commensurate with an approach producing high end estimates of predicted environmental concentrations.

2.1.6 Quantifying consequences, likelihood and risk

Commensurate with the impact and risk analysis method developed for the Bioregional Assessments Programme (Barrett et al. 2013), the National Coal Seam Gas Chemicals Assessment methodology will determine consequences or impacts of drilling and / or hydraulic fracturing chemicals on human health and the environment, and the likelihood of impacts on receptors contained within receiving environments based on the propagation of uncertainties from models and data. The impact analysis is influenced by a number of factors that affect the method adopted. The methods should be practical and suittable for adoption in the region under study given data, time and financial resources available. The nature of the impacts, the availability and quality of data, and the available capability and skills to undertake an analysis all influence the methods adopted. Methods used within the National Coal Seam Gas Chemicals Assessment for impact analysis include conceptual models (this report) and numerical modelling of direct impacts (Mallants et al. 2017b).

2.2 Potential release of chemicals associated with coal seam gas operations to the environment: soil and shallow groundwater pathways

The lifetime of an individual coal seam gas well or an entire coal seam gas well field can be divided into different phases (Figure 2.5). Each phase has a number of typical activities with a relatively well-defined duration and set of risks. Importantly, these risks are not equally distributed across time and space.



Note. Duration of each phase is indicative (length of arrows is not to scale).

Figure 2.5 Phases of development and operation of a coal seam gas project with typical activities

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 per coal seam gas well.
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

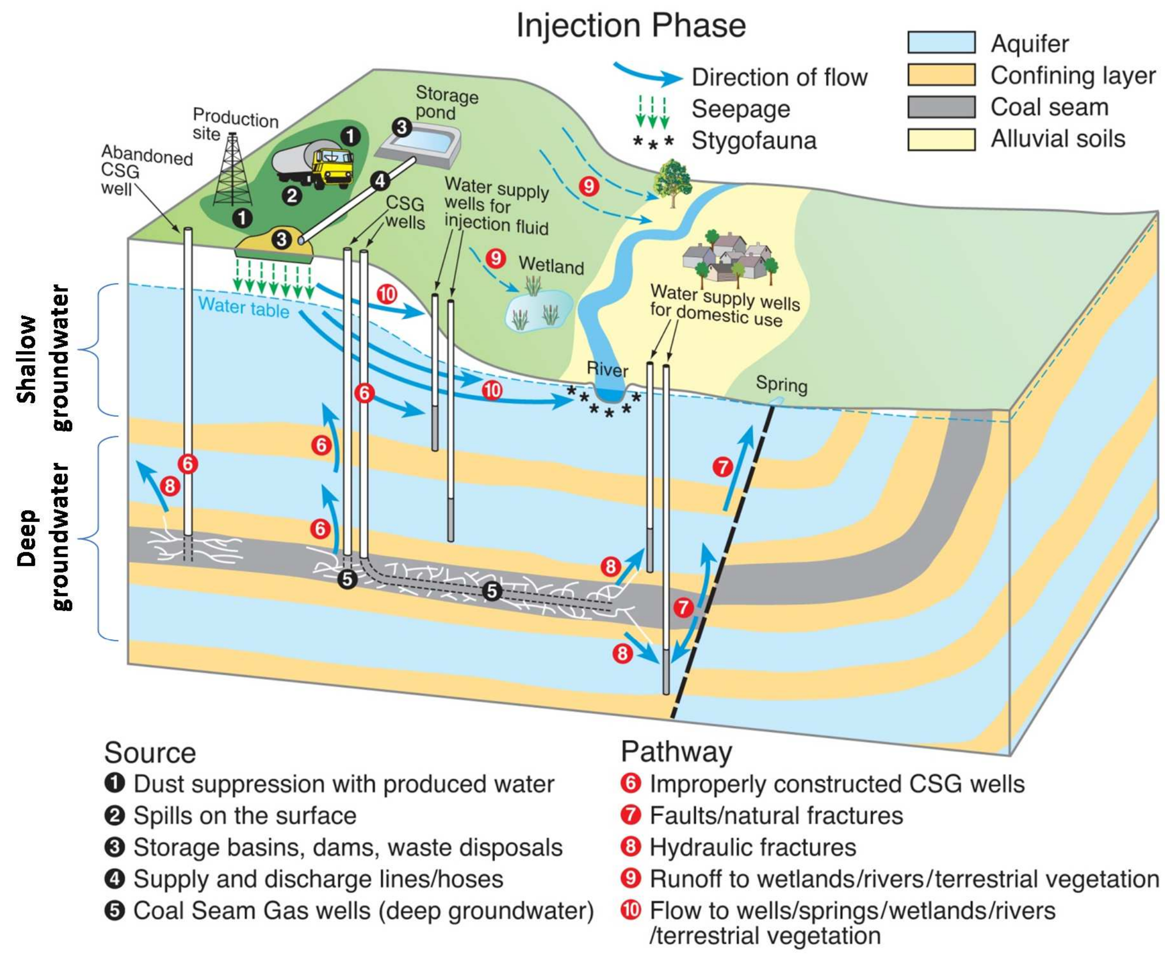
Surat Basin (Queensland), and as a result, hydraulic fracturing will likely have greater application in the Bowen Basin than in the Surat.

4. Depressurisation 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 depressurised, gas flow rates continue to rise to a peak rate (months or years after dewatering started) and water flow rates decline. There may be a number of depressurisation events intermittent with injection phases. The total duration of the depressurisation phase may be up to 20 or 30 years.
5. Return to equilibrium or post-operational phase: starts at the end of the depressurisation 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 depressurisation. In other words, although the depressurisation 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 easily in excess of 100 years (AE 2012a), and might in some circumstances take a thousand years or longer to reach a new equilibrium (CH2MHill 2013).

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 previously been summarised by Mallants et al. (2017a). In the following discussion we focus on potential releases of chemicals used or produced during the pressurisation/injection, depressurisation, and return to equilibrium phases.

As part of the consideration of environmental impacts associated with coal seam gas operations within the pressurisation, depressurisation, and return to equilibrium phases, there is concern about the potential for contamination of 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 (see, e.g. Brantley et al. 2014):

- 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 Source: CSIRO (Mallants et al. 2017a)
- Figure 2.6 for injection phase and
- Source: CSIRO (Mallants et al. 2017a)
- Figure 2.7 for depressurisation phase).



Note. Source 5 and pathways 6–8 are not considered for shallow groundwater exposure assessments.

Source: CSIRO (Mallants et al. 2017a)

Figure 2.6 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)

During the depressurisation 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 (Source: CSIRO (Mallants et al. 2017a)

Figure 2.7).

- Infiltration of flowback and produced water into soil due to use of this water for dust suppression at a site (Source 1). 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 2). 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 groundwatertable. 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, and hazardous events including flooding (Source 3) (The Royal Society and The Royal Academy of Engineering 2012). In Australia design requirements for storage basins include the bottom of the basins being sealed with a clay liner or a material such as a geomembrane with an equivalent low permeability of 5.2 cm in 15 years which translates to a maximum hydraulic conductivity of ~ 10^{-10} m/s (AE 2008; DITR 2007). Seepage may occur through the basin floor or containment wall. Overtopping or dam flooding as a result of extreme rainfall events is another potential pathway for chemical release.
- Releases from supply and discharge lines and hoses that transport produced water from the well site to the storage ponds (Source 4). 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.

The potential pathways for contaminant transport of fluids associated with hydraulic fracturing operations at the coal seam gas site (pathways 9 to 10 in Source: CSIRO (Mallants et al. 2017a)

Figure 2.7) include:

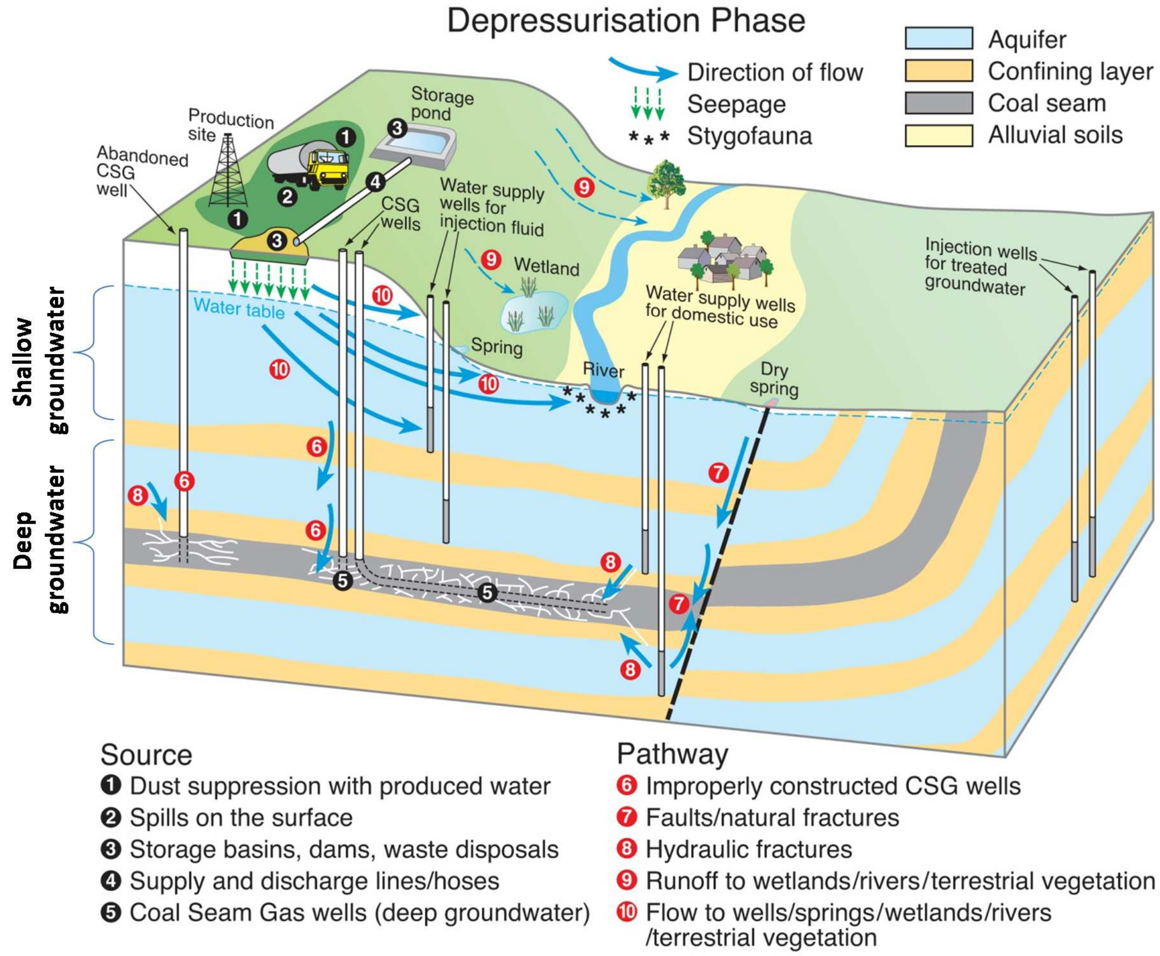
- runoff to wetlands and rivers. This includes the potential flow of spilt chemicals on the land surface to water courses (for conceptual models at the land surface see DoEE 2017b)
- subsurface flow from surface sources to wells, springs, wetlands, and rivers. The potential flow includes unsaturated zone flow and saturated zone flow, and surface sources (1 to 4), as discussed above. Additional receptors of potentially contaminated groundwater include groundwater dependent terrestrial vegetation and, mainly along rivers with interconnected unconsolidated alluvial aquifers with a high porosity, stygofauna (AE 2012b). Consideration of terrestrial vegetation and stygofauna in the environmental risk assessment will depend on availability of relevant ecotoxicological data.

Discussions about the potential pathways for solute transport in deeper groundwater (pathways 6, 7 and 8 in Source: CSIRO (Mallants et al. 2017a)

Figure 2.6 and Source: CSIRO (Mallants et al. 2017a)

Figure 2.7) and their potential impacts are beyond the scope of this exposure assessment.

Assessment of the impact of chemical releases from a coal seam gas site to the environment requires the following components: source model, pathway or transport model, and response model. The source model describes the composition of the contaminant source and the rate at which it is released into the soil (the soil is the first component of the landscape likely to be in contact with the emission sources 1 to 4). A source model can be a very simple uniform release rate as a function of time; it may be a continuous decreasing release function to represent biodegradation or increased dilution in the pond, or it can be a more complex function to represent a combination of processes that result in a complex evolution of contaminant concentrations (see Section 3 for details).



Note. Source 5 and pathways 6–8 are not considered for shallow groundwater exposure assessments.

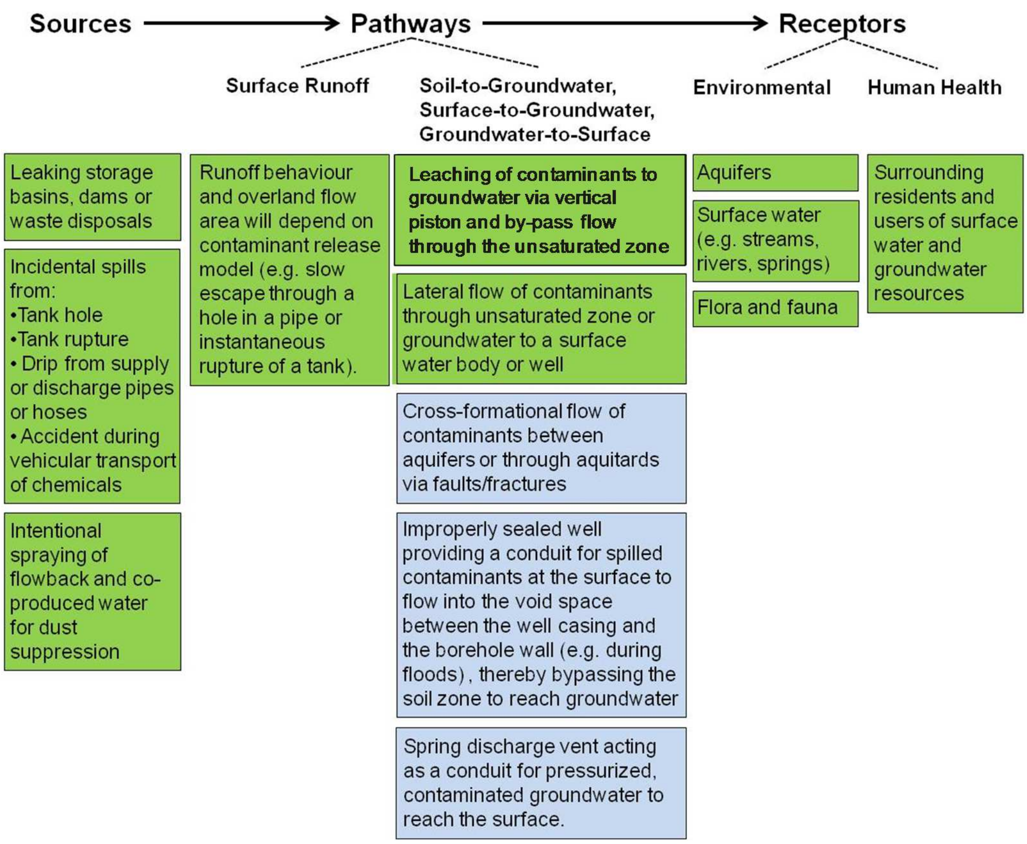
Source: CSIRO (Mallants et al. 2017a)

Figure 2.7 Possible contaminant sources at the coal seam gas site (1 to 5) and pathways for solute transport during the depressurisation phase (6 to 10).

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 (Figure 2.8). 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.

A contaminant transport model describes the amount of chemicals in a given (soil or groundwater) location (contaminant concentration) and the rate of migration (contaminant flux) at a given time along the solute’s pathway from source to receiving environment (see pathways 9 to 10 in Source: CSIRO (Mallants et al. 2017a)

Figure 2.7). Subsurface pathways for spills and leaks include the soil-to-groundwater pathway (e.g. leaching of contaminants to groundwater via vertical migration through the unsaturated zone or lateral migration of contaminants through either the unsaturated zone or saturated zone) and the groundwater-to-surface pathway (e.g. spring, stream and wetland discharge; Figure 2.8). In the remainder of this study the latter two will be combined into a single groundwater pathway.



Note. The boxes shaded in green are within the scope of this study, whereas the boxes shaded in blue refer to deep groundwater and are not in the scope.

Figure 2.8 Source-pathway-receptor analysis for contamination derived from spills and leaks

The response model quantifies the impact of one or several contaminants, sometimes in combination with other stressors such as temperature, on human health or fauna/flora species. The following receiving environments or receptors are considered relevant in the framework of this exposure assessment: soil and its ecosystems (mainly plants), groundwater, groundwater wells, streams, wetlands and springs (for a summary see Table 2.1). Surface water pathways are considered elsewhere (DoEE 2017b, 2017c).

Table 2.1 Pathways for solute migration in soil and shallow groundwater, their receptors and computational endpoints to be considered in this study

Pathway	Receiving environment	Description	Computational endpoints
Soil-to-groundwater	Soil and soil ecosystems	Solute is transported from a surface source into soil (unsaturated zone) and potentially becomes a risk for soil ecosystems, soil biodiversity, and plants	Solute concentration in soil water; solute flux at soil / groundwatertable interface
Soil-to-groundwater	Groundwater	Solutes reach the groundwatertable,	Solute flux at soil/groundwatertable

Pathway	Receiving environment	Description	Computational endpoints
		become mixed with the shallow groundwater, and develop a plume which migrates within flowing groundwater and can be intercepted by deep-rooted plants	interface; solute concentration in groundwater with minimum dilution (assuming well is within the source area); unsaturated zone dilution factor (DF_L)
Groundwater	Well	Solute plume is intercepted by an irrigation or drinking water well	Solute concentration in groundwater at location of a well; groundwater dilution factor (DF_{GW}); travel time from bottom of unsaturated zone to well location
	Stream	Solute plume is intercepted by the gaining section of a stream; solutes are further diluted in the stream	Solute concentration in surface water at location where plume discharges; surface water dilution factor (DF_{SW}); solute flux into stream; travel time from bottom of unsaturated zone to stream
	Wetland	Solute plume is intercepted by a wetland; solute accumulation occurs in the wetland	Solute concentration in wetland at location where plume discharges; solute flux into wetland; travel time from bottom of unsaturated zone to stream
	Spring	Solute plume is intercepted by discharge flowing to a spring; solute accumulation occurs in the spring zone	Solute concentration in spring discharge; solute flux into spring zone; cumulative flux into spring; travel time from bottom of unsaturated zone to stream

3 Coal seam gas operations and identification of contaminant source characteristics

3.1 Physical and chemical characteristics of potential contaminants

The critical physical and chemical characteristics of potential contaminant sources associated with coal seam gas operations at the surface that are needed to conduct exposure assessments include:

- the surface area through which potential leakage into the subsurface may occur, with the three main geometries being classified as point, line and areal sources
- the volume of fluid that potentially leaks into the underground. Two types of leakage scenarios are considered: a spill with a fixed volume of contaminated water (the duration of infiltration depends on the infiltration capacity of soil), and a leak of a fixed duration (the infiltrated volume depends on leakage rate)
- the duration of a potential leakage (a single short pulse of typically one day or long-term steady leakage for several years), and possibly the frequency of occurrence for multiple events
- the chemical composition of the fluids. For details on the chemical composition, the reader is referred to the *Identification of chemicals associated with coal seam gas extraction in Australia* report (NICNAS 2017c)
- the concentration of chemicals (Table 3.1).

Source characteristics were previously determined by Mallants et al. (2017a) on the basis of a literature review. A summary is provided in Table 3.1 and serves as the basis for deriving physical (Table 3.3) source parameters used in the solute transport simulations for the soil pathway.

Table 3.1 Summary of source characteristics (surface area involved for a point source is estimated and assumed to be roughly proportional to volume of fluid released)

Source type	Surface area involved	Maximum volume of fluid assumed to be released	Duration of release	Chemical composition	Concentration of chemicals
Point sources					
Flat-bed trucks loaded with containers (HFF)	~ 10 m^2	220 gallons to 375 gallons (i.e. 833–1 420 L) HDPE totes	Instantaneous	Various; liquid additives.	See NICNAS (2017c)
Flat-bed trucks loaded with	~ 1 m^2	One gallon (i.e. 3.8 L)	Instantaneous	Various	See NICNAS

Source type	Surface area involved	Maximum volume of fluid assumed to be released	Duration of release	Chemical composition	Concentration of chemicals
containers (HFF)		jugs			(2017c)
Flat-bed trucks loaded with containers (HFF)	~ 1 m^2	Five gallon (i.e. 19 L) sealed buckets	Instantaneous	Various	See NICNAS (2017c)
Tanker truck (HFF)	~ 10 m^2	Contents of the tanker truck (e.g. 4 000 gallons; 15 142 L)	Instantaneous	e.g. Hydrochloric acid	See NICNAS (2017c)
Line sources					
Leaking pipes of produced water transported to water treatment facility	Few 100s of m^2 (based on a 1×100 m contaminated area)	Several m^3	Instantaneous and long-term (if not immediately detected)	Various	Uncertain; refer to typical concentrations in flowback water as a guide (see NICNAS 2017c)
Leaking hoses from blender truck to well (fracturing)	Few 10s of m (based on a 1×10 m^2 contaminated area)	Several m^3	Instantaneous	Various	Uncertain
Area sources					
Dust control	Up to 1 ha	10 000 L/day/ha or 10^{-3} m/m^2/day	Up to one year	Depending on groundwater geochemistry and degree of interaction with HFF	Uncertain; refer to typical concentrations in flowback water as a guide (see NICNAS 2017c)
Storage ponds for flowback and produced water	Various sizes (e.g. 1600 m^2 and larger)	Normal operations with clay liner: estimated leakage rate of 10^{-10} m/s or 32 m^3/ha/y (max. permissible leakage rate) Accidental conditions (e.g. flooding): several orders of magnitude	Long-term (years)	Depending on groundwater geochemistry and degree of interaction with HFF	Uncertain; refer to typical concentrations in flowback water as a guide (see NICNAS 2017c)

Source type	Surface area involved	Maximum volume of fluid assumed to be released	Duration of release	Chemical composition	Concentration of chemicals
		higher Improper rehabilitation after cessation of coal seam gas activities			
On-site evaporation ponds	Various sizes (up to several ha)	Normal operations with clay liner: estimated leakage 10^{-10} m/s or 32 m^3/ha/y Accidental conditions (flooding): several orders of magnitude higher	Long-term (years)	Depending on groundwater geochemistry and degree of interaction with HFF	Uncertain; refer to typical concentrations in flowback water as a guide (see NICNAS 2017c)

Note. HFF refers to hydraulic fracturing fluids.

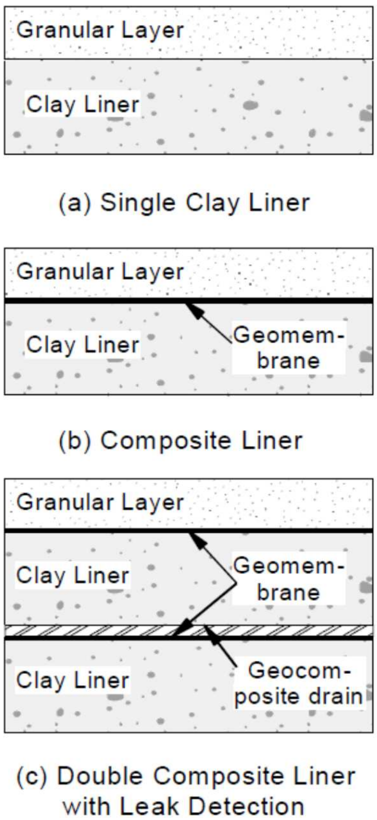
The potential volumes considered under the heading of point sources are of the same magnitude as those considered by DoEE (2017b), i.e. DoEE considers 20 L, 206 L, and 500 to 1 000 L containers and 10 000 L or larger trucks. The relatively small differences in volumes used in this exposure assessment do not materially affect the outcome of the calculations of chemical concentrations in receiving environments.

3.2 Potential source volumes and leakage rates

In defining potential source volumes and leakage rates, a distinction is made between a spill and a leak. In a leak situation, it is assumed that there is entry of fluid into the subsurface soil under well-defined conditions of time and space (Simon and Keller 2003). The main variables defining the release of chemicals associated with a leak are the leak area, duration and the rate of entry. In contrast, in a spill situation (such as a tank hole, tank rupture, a drip from hoses or pipes, accident involving a vehicle transporting chemicals), there can be overland flow and concurrent infiltration and evaporation of the fluid (Simon and Keller 2003). The spreading area associated with a land surface spill must be defined and is strongly controlled by the release rate of a spill and by the subsurface permeability (Simon and Keller 2003). To model a spill, the volume of spill and the affected area must be known.

Produced water is stored in surface ponds before being either re-used (agricultural, urban, and industrial uses) or treated on-site or off-site. Lined ponds are known to leak over time even when double lined (Chapuis 2002; Council of Canadian Academies 2014). Furthermore, the salinity of the stored produced water can increase the permeability of clay-lined ponds (Folkes 1982; Benson 2001).

Lining systems can vary considerably in complexity (Figure 3.1). The simplest lining systems consist of a compacted clay liner, a geosynthetic clay liner (GCL), or a geomembrane[2] (GM) liner overlain by a granular collection layer (Figure 3.1a). A more sophisticated and effective lining system incorporates a composite liner (Figure 3.1b) comprised of a GM placed directly on top of a clay liner (or other type of soil liner). The most effective design considers a double composite liner with a leak detector and / or leachate collection system (Figure 3.1c).

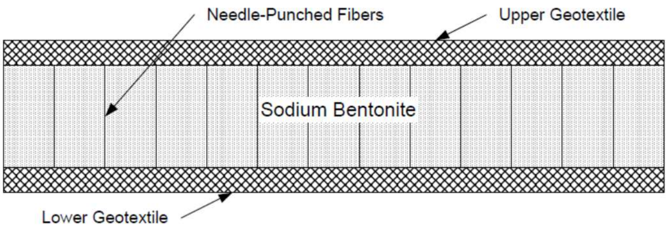


Source: Benson (2001)

Figure 3.1 Compacted clay liner with granular leachate collection layer (a), composite liner with granular leachate collection layer (b), and double composite liner with upper granular leachate collection layer and lower geo-composite leak detection layer (c).

A GCL (typically < 10 mm thick) is a relatively thin layer of several mm of processed clay (typically sodium bentonite) either bonded to a geomembrane or fixed between two sheets of geotextile (Figure 3.2). Advantage of GCLs over traditional clay liners is that they are easy to install, have a low hydraulic conductivity and they have the ability to selfrepair holes upon contact with leachate water, caused by the swelling and self-healing bentonite. Laboratory tests demonstrated that they can heal holes up to 75 mm. Laboratory tests have further demonstrated that dry, unconfined bentonite has a hydraulic conductivity of 10^{-11} m/s; when saturated, this value may drop to 10^{-14} m/s (US EPA 2001).

[2] Typically 1.5 to 2.5 mm thick high density polyethylene



Source: Benson (2001)

Figure 3.2 Schematic of a common GCL with two carrier geotextiles that are needle-punched together to retain the bentonite and provide greater internal shear strength.

Composite liners are the most common liners used for municipal solid waste (MSW) landfills in North America, Europe, Australia, and New Zealand (Benson 2001). Current engineering practices for lining landfills and storage ponds consider double liner systems which incorporate leakage collection systems. Figure 3.3 considers three typical designs: a double compacted clay liner (CCL) system, a double geosynthetic clay liner (GCL) system, and a single GCL underlain by an attenuation layer (Rowe 2010).

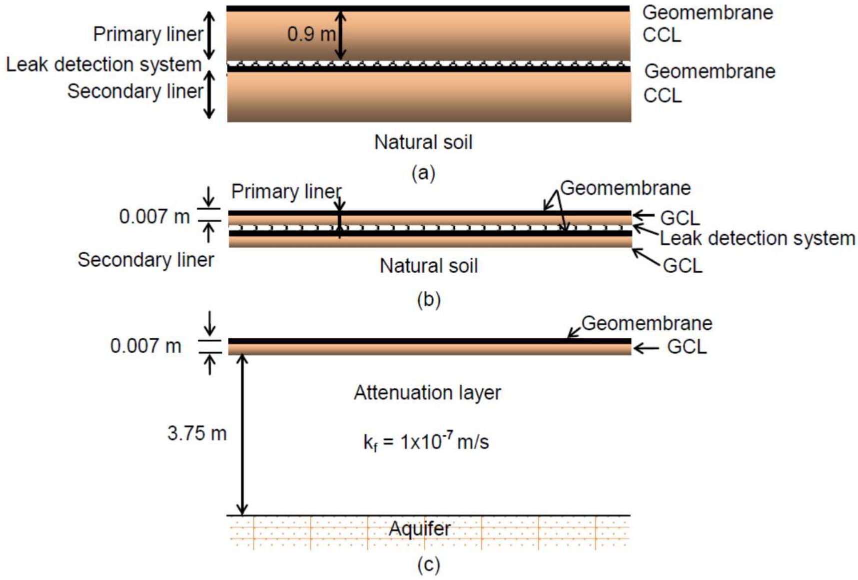
While generally low, leakage (the combination of advective and diffusive migration of fluids) from a composite liner (GM combined with either a CCL or a CGL) cannot be avoided and is mainly due to the fact that a GM installed as part of liner system will generally have some holes (2.5 to 5 holes per hectare being most commonly assumed (Rowe et al. 2004; Rowe and Hosney 2010; Rowe 2012). According to Rowe (2012) holes may form as a result of:

- manufacturing defects
- handling of the GM rolls
- on-site placement and seaming
- cleaning of residue from a water holding pond
- stress cracking as the GM ages.

Leakage from a single GM with 2.5 holes per hectare (leakage head or water depth of 5 m typical of a water holding pond) was calculated to be 1 000 lphd[3] (1.2×10^{-9} m/s) and 4 000 lphd (4.6×10^{-9} m/s) for 0.5 and 1 mm radius holes, respectively (Rowe 2012). Evidence compiled by Rowe (2012) indicates that under normal operating conditions, the GM service life can be very long, up to thousands of years.

Composite liners such as those in Figure 3.3 provide a means of minimizing the leakage, as was demonstrated by Bonaparte et al. (2002) based on field observations. Compared to a GM/CCL composite liner (Figure 3.3a), a GM/GCL composite (Figure 3.3b) reduces leakage typically by factors ranging from one to two orders of magnitude: from 50 lphd (water flux of 5.8×10^{-11} m/s or 1.825 mm/year) for a CCL to 0.6 lphd (water flux of 7×10^{-13} m/s or 0.022 mm/year) for a GCL (mean values). This provides empirical evidence for superior performance of GCLs compared to CCLs in composite liners. The superior performance of CGLs is mainly due to their intrinsically lower hydraulic conductivity, typically between 2 to 5×10^{-11} m/s (Rowe and Hosney 2010, Rowe 2012), and their ability to selfrepair holes.

[3] lphd = litres per hectare per day



Source: Rowe (2010)

Figure 3.3 Schematic of typical double liner systems: (a) Primary composite liner with compacted clay liner (CCL), H_L=0.9 m, (b) Primary composite liner with geosynthetic clay liner (GCL), H_L=0.007 m, (c) Single composite liner with GCL (H_L=0.007 m) on a 3.75 m thick attenuation layer underlain by an aquifer. H_L is thickness of CCL or GCL; K_f is hydraulic conductivity.

The leak rates discussed above are obtained from municipal landfills which typically have a small head of leachate water on top of the composite liner (a commonly used design value is 0.3 m, Rowe and Hosney 2010). Rowe and Hosney (2010) demonstrated that a leachate head of 4 to 5 m would increase the leak rate by about one order of magnitude. For produced water holding ponds, water heads of 4 to 5 m are common. For a discussion on specific issues regarding liner performance for water holding ponds the reader is referred to Rowe (2012). Effects of water salinity on the permeability of GCLs are significant for 0.1 to 1 M solutions: compared to permeability for deionized water (approximately 2×10^{-11} m/s), 0.1 M NaCl increases permeability by about one order of magnitude (2×10^{-10} m/s) whereas at 1 M NaCl the increase can be up to 10^{-6} m/s (Benson 2001).

Further useful information regarding leak rates and their likelihood is provided in Beck (2012a; 2012b) based on leak rates for double-lined landfills in the US. Comparison of likelihood of leak rates is based on a 1992 survey of 14 landfill cells and a 2012 survey of 128 landfill cells. The leakage rates were obtained from measurement of leakage through the primary geomembrane collected and quantified in the secondary containment system.

Table 3.2 provides the probability of exceeding a specified leakage rate for the two surveys: owing to advances in installation quality and construction quality assurance practices, leakage rates greater than 50 lphd have decreased significantly in the past 20 years. The observation that 73% of the 2012 landfills had leakage rates less than 50 lphd (5.8×10^{-11} m/s) is consistent with the leakage rates for composite liners (from 50 lphd for a CCL to 0.6 lphd for a GCL) reported by Rowe (2012).

Table 3.2 Distribution of average landfill leakage rates.

Leakage rate			**Percent of landfill cells**	
lphd	***m/s***	***mm/year***	**1992**	**2012**

< 50	< 5.8×10^{-11}	< 1.825	43%	73%
50–200	5.8×10^{-11}–2.3×10^{-10}	1.825–7.3	36%	24%
200–500	2.3×10^{-10}–5.8×10^{-10}	7.3–18.25	14%	3%
500–1000	5.8×10^{-10}–1.2×10^{-9}	18.25–36.5	7%	0%
>1000	> 1.2×10^{-9}	> 36.5	0%	0%

Note: lphd = liters per hectare per day

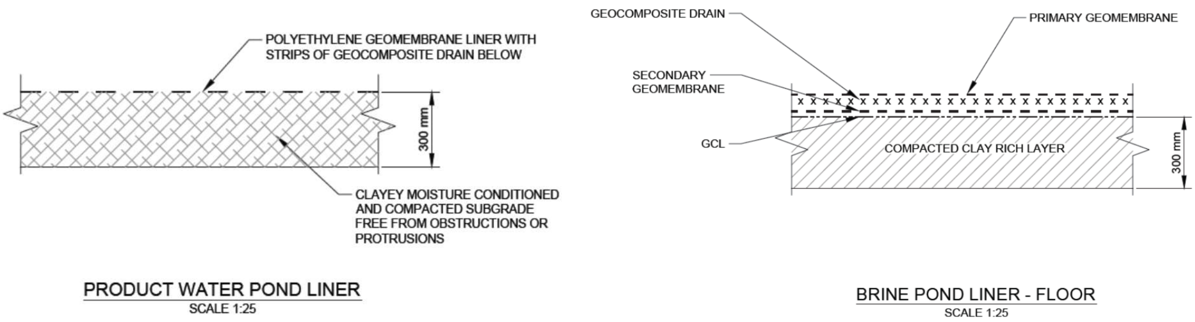
Source: Beck (2012a)

In a survey of regulations regarding maximum allowable leakage from liquid impoundments adopted by US governmental agencies et al. (Koerner and Koerner 2009) concluded that i) for sewage and wastewater ponds the maximum allowable leakage varied between 130 to 34 000 lphd (based on 37 state agencies), ii) the Interagency Wastewater Committee of the Great Lakes/Upper Mississippi River Board of State and Provincial Public Health and Environmental Managers imposed a maximum leakage rate for wastewater collection and treatment facilities of 5 000 lphd.

In Australia design requirements for storage basins are stipulated by the Queensland Department of Environment and Resource Management “Manual for Assessing Hazard Categories and Hydraulic Performance of Dams” (DERM 2012) and the NSW Dam Safety Committee (DSC) requirements (NSW Government 1978). Further relevant guidance regarding liner design may be obtained from DITR (2007) for tailings management; a compacted clay liner would normally be expected to achieve a saturated hydraulic conductivity of less than 10^{-8} m/s. A geomembrane would be expected to achieve an equivalent hydraulic conductivity of approximately 10^{-10} m/s, a value that is approximately 10 times lower than the leakage calculations from Rowe (2012) — see higher.

Several different liner designs exist across the storage ponds used to manage coal seam gas produced water in Australia.

- Arrow’s evaporation dams for produced water in Dalby have a clay liner or a material such as a geomembrane with an equivalent low permeability of 5.2 cm in 15 years (AE 2008), which translates to a maximum hydraulic conductivity of about 10^{-10} m/s. This is a single layer design similar to that in Figure 3.1a.
- Santos uses single composite liners for its Leewood Ponds in Narrabri, NSW (Source: RPS (2012)
- Figure 3.4). The produced water pond liner has a GM on top of a 300 mm clayey subgrade, while the brine pond liner has a primary and secondary GM with a geocomposite drain in between, and a GCL on top of a 300 mm compacted clay rich layer.
- Designs by Clarke (2008) for coal seam gas exploration activities in Stratford (NSW) indicate a single geomembrane as liner for its temporary water holding ponds.



Source: RPS (2012)

Figure 3.4 Liner designs for Leewood Ponds, Narrabri NSW (RPS 2012)

The selection of a leak rate for exposure calculations is considered to represent normal operations of the storage pond, i.e. a performance that is at least as good as the design specifications and possibly better. The selected leak rate has to account for various factors, including the variation in liner designs across the Australian landscape, the uncertainty about the leak rate for a specific liner design, and the advances in installation quality and construction quality assurance practices yielding better performing liners (Table 3.2). Therefore, a range of leak rates is considered rather than a single “best estimate” leak rate. Three leak rates are selected for exposure calculations: 0.35, 3.5 and 35 mm/year. The range 0.35 to 35 mm/year approximately corresponds with the range proposed by Beck (2012a) as summarised in

Table 3.2:

- 0.35 mm/y (~10^{-11} m/s) corresponds to the < 50 lphd class with a probability of 73% (2012 survey). The 0.35 mm/y leak rate has a much higher likelihood than the two other values and could be considered a reference value for designs that include a GM/GCL composite liner.
- 3.5 mm/y (~10^{-10} m/s) corresponds to the 50-200 lphd class with a probability of 24% (2012 survey). The 3.5 mm/y leak rate on the other hand is more representative of a GM or CCL composite liner (see discussion above).
- 35 mm/y (~10^{-9} m/s) corresponds to the 500-1 000 lphd class with a probability of 0% for the 2012 survey and 7% for the1992 survey. The 35 mm/y leak rate is typical for a design with a single GM liner, or a compacted clay liner if sufficiently thick (see higher).

These three classes assume a single liner system (i.e. a single composite liner); in case of a double liner system (see Figure 3.3), the leak rates can be expected to be even smaller. It is further important to note that the three classes of leak rates selected here represents a very slow, diffuse but long-term leakage rate across the entire pond under normal operation. This is different from considering an accidental leak, in which case much higher fluid rates exist. From a preliminary assessment of a real breach in a pond liner presented in Mallants et al. (2017b) it is demonstrated that much higher leak rates exist than the 10^{-10} m/s considered here. However, such high leak rates usually occur only over a limited surface area of the pond and the loss of considerable volumes of water generally leads to timely detection and subsequent remediation.

Table 3.3 summarises the physical characteristics of surface sources that will be considered in the exposure assessments. For each of the three characteristics (surface area, source volume and leakage duration), a range of values is proposed to account for the often large variation in such characteristics. The conceptualisation considers a leak duration of either 3 or 30 years. The 3-year leak is considered for those cases where produced water is stored for a well “appraisal” period assumed to last up to 3 years. These ponds are typically located nearby the coal seam gas production wells. For example, Santos considers so-called appraisal pilots to manage pilot water production near Narrabri (NSW) for a period up to 3 years (RPS 2012). Shorter appraisal periods up to one year have also been considered (Clarke 2008). The 30-year leak duration is relevant for the entire coal seam gas productive phase; given that the design life of the storage ponds for produced water is typically 25 to 30 years, the selection of a 30-year leak duration is justified. Such ranges are based on the values obtained from the literature review (Table 3.1).

Table 3.3 Physical characteristics of surface sources considered in exposure assessments

Surface area		Volume		Duration	
		Spill	***Leak***	***Spill***	***Leak***
Point source	[1, 10] m^2	[3.8, 15 000] L		*K*-dependent	
Line source*	[10, 100] m^2	-	[10, 10 000] m^3	-	[1, 100] days
Area source	10 ha	-	35 m^3/y for leak rate of 3.5 m^3/ha/y§	-	3, 30 years
Area source	10 ha	-	350 m^3/y for leak rate of 35 m^3/ha/y$^\$$	-	3, 30 years
Area source	10 ha	-	3 500 m^3/y for leak rate of 350 m^3/ha/y$^\#$	-	3, 30 years

*Numbers in brackets are ranges. * from 10 to 100 m long and a unit width of 1 m (leak rate of 1 m^3/day); §equal to 0.35 m/y; $^\$$ equal to 3.5 m/y; $^\#$ equal to 35 mm/y.*

4 Groundwater model selection

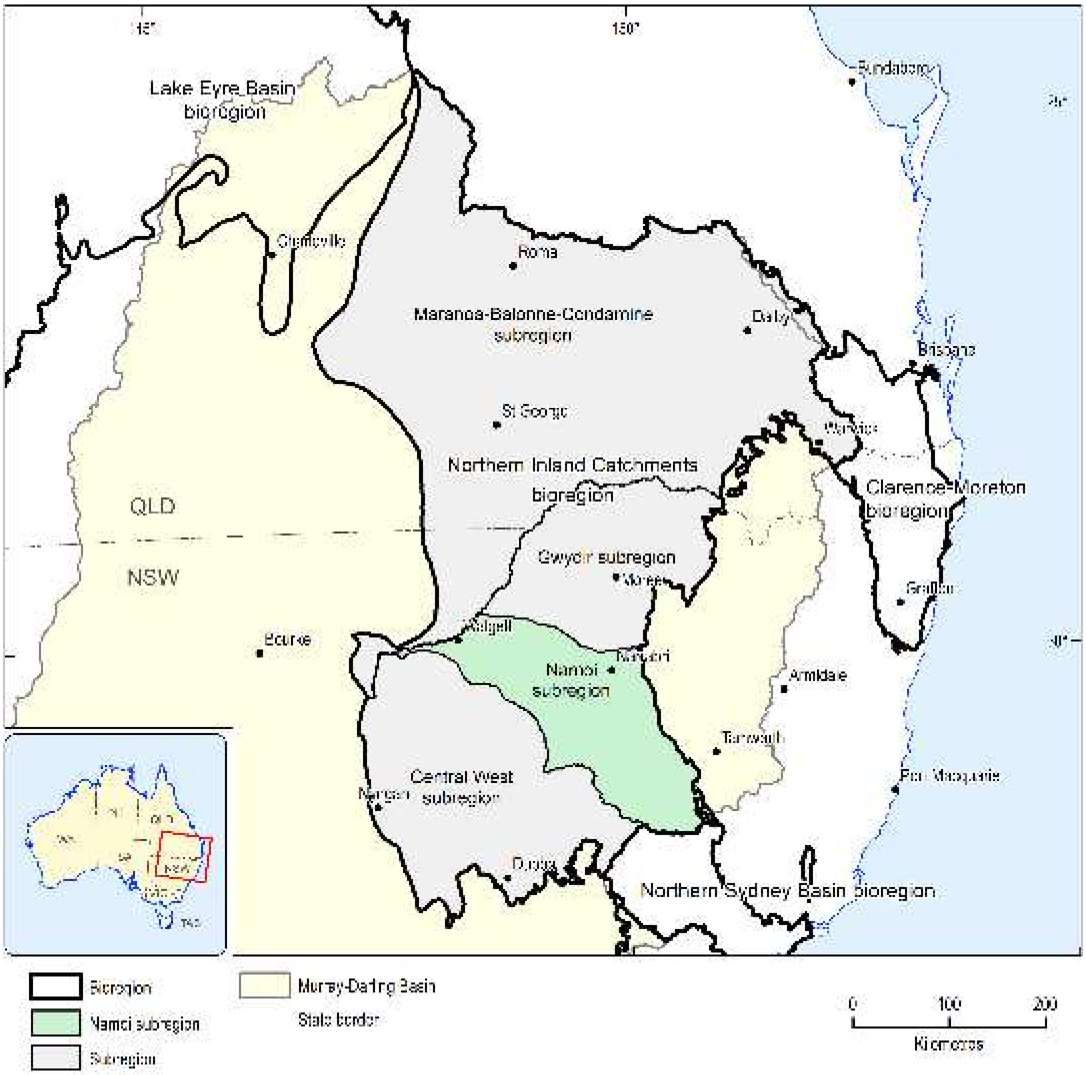
4.1 General background information on Namoi catchment

The Namoi catchment region located in north-eastern New South Wales was selected for this study due to its location in one of the subregions of the Northern Inland Catchments (Figure 4.1) that were identified for bioregional assessments (IESC 2013). The Namoi valley is a major agricultural area which is used extensively for growing irrigated crops including barley, wheat, sorghum, soy and cotton (Ashton et al 2011; Welsh et al. 2014). It has also been intensively developed for groundwater resources (see Section 5.3.2.3). In several areas of the catchment coal seam gas exploration and extraction occurs (Figure 4.1). Although hydraulic fracturing as part of coal seam gas extraction is not current practice in the Namoi, it cannot be excluded as part of future extraction (Lewis 2014). The region has one of the highest levels of groundwater extraction within the Murray-Darling Basin (MDB) and groundwater use is 15.2 per cent of the MDB total (CSIRO 2007). Annual groundwater use between 2008 to 09 and 2012 to 3 has been considerably lower than the early 2000s, ranging from approximately 30 to 80 GL (Welsh et al. 2014). The catchment is home to approximately 100 000 people concentrated mostly along the Namoi River and its tributaries between Tamworth and Narrabri.

Due to rising concerns within the community that coal seam gas development will impact catchment water resources, the NSW Government commissioned the Namoi Catchment Water Study in August 2010 (SWS 2012b). This study involved development of a three-dimensional numerical model to predict the potential impacts of different mining (open cut and underground) and gas developments on water resources. The study progressed in four phases, ending with a final phase in July 2012 (SWS 2012b). The four phases were:

1. scoping and literature review (SWS 2010)
2. data collation, analysis and conceptualisation (SWS 2011)
3. modelling (SWS 2012a)
4. final reporting (SWS 2012b).

Impacts from coal seam gas extraction on groundwater mainly occur within the coal seam measures (in the Namoi catchment these are the Black Jack and Maules Creek Formations) where pumping groundwater out of the coal reduces the fluid pressure within and near the coal seams (depressurisation or drop in hydraulic head) (SWS 2012b). As a result, methane gas is desorbed and released from the coal (higher ambient water pressure ensures that a higher proportion of methane at any location within the coal remains adsorbed to the coal). The degree to which depressurisation is translated to overlying or underlying aquifers, and its timing, depends on the spatial distribution of hydraulic connectivity, both horizontally within hydrostratigraphic units and vertically across them. When tight formations (aquitards) isolate the coal seams, impacts on other aquifers, including shallow groundwater aquifers, are likely to be limited, at least in the short term. Assessment of the impact of coal seam gas extraction on groundwater resources requires a validated groundwater model of the deep coal seam gas coal seams, the overlying and underlying formations, and sometimes including connections with alluvial aquifers and their interactions with streams (Commonwealth of Australia 2014).



Source: Commonwealth of Australia (2014)

Figure 4.1 Location of the Namoi catchment in NSW relative to the Northern Inland Catchments

A description of the potential impact of open-cut mining on water resources is provided by Smith (2009). Through excavation and dewatering, open-cut mining can have impacts on streams, aquifers and alluvial soils. The associated pit infrastructure intercepts, and then captures, rainfall and runoff. Mining below the watertable can have an impact on groundwater resources due to depressurising, inducing local changes in groundwater gradients and flow directions. Underground mining induces groundwater flow in a similar way. This water needs to be managed, either by intercepting it before it reaches the mine (via dewatering wells) or using in-pit sumps or wells. This will have an impact on the local groundwater system. The direct effect of underground mining on surface water features is generally less than that caused by open cut mining, due to the smaller surface expression of the mine and reduced area of surface water management. Current coal mining exploration and activity prospects are limited to a zone through the centre of the catchment which closely follows the location of the alluvial deposits upstream of Narrabri. The Namoi Catchment Water Study study and its associated catchment model focused on the alluvial aquifers in close proximity to both potential and existing coal and gas operations and Gunnedah Basin sediments intersected by coal and gas operations. Assessment of impacts of mining on water resources therefore requires groundwater models of the alluvial aquifers and their interactions with streams (Welsh et al. 2014; Lewis 2014).

As the Namoi Catchment Model (NCM) produced by SWS is recent, well documented, and has a rigorously tested alluvial aquifer model component (SWS 2011), it was selected for adaption and use in evaluating environmental concentrations of chemicals associated with spills and leaks. The alluvial groundwater model has a fairly coarse grid size (plan view) of 1×1 km^2, with several regions with very good model performance (see further Section 5.3). These regions are relevant for the exposure assessment of chemicals leaking from the soil surface into shallow groundwater. In these regions the model can be relatively easily adapted to fit the requirements for solute transport simulations. A brief summary of the conceptual underpinnings of the NCM is provided herein to provide a background context.

4.2 Fitness-for-purpose

The NCM developed by SWS has a number of assumptions that were taken into consideration in adapting it for the current conceptual pathway models for human and environmental exposures to HFF spills and leaks. Some of the critical assumptions for the numerical model are listed in Table 4.1 (SWS 2012a, 2012b). None of them have a significant impact on the current exposure assessments. It is important to note that the area of highest data coverage within the geological model domain (SWS 2012a) coincides with the two sub-model domains evaluated in this study.

Table 4.1 Assumptions about the NCM and their relevance to the current exposure Assessment

Model assumptions	Relevance for current assessments
Groundwater flow is assumed to be within porous media (unconsolidated sediments or rock); dual porosity and fracture flow were not simulated.	For flow and transport simulations in the alluvial aquifers composed of sands, gravels and clays, the assumption of a single porosity medium is sufficient as such materials are generally characterised by a single pore-size distribution.
Single phase conditions (no gas phase around coal seam gas wells)	When only shallow groundwater is considered for solute transport, existence of a gas phase in the groundwater (multiphase flow) is irrelevant. Multi-phase flow (presence of a water and gas phase) would typically exist in the coal seams around a coal seam gas well as a result of depressurisation and subsequent gas release and formation of a pure gas phase. Since such multi-phase flow conditions generally do not exist in the shallow groundwater, the groundwater model will reflect all relevant processes. In shallow groundwater a gas phase does exist but only above the groundwatertable, which is in the unsaturated zone. The unsaturated zone is treated separately by a modelling approach that accounts for effects of such gas phase on unsaturated water flow and solute transport.
No fluid density effects	Fluid density effects as a result of saline groundwater are not important for the very shallow groundwater (the likely range of salinities encountered in the aquifers is unlikely to result in fresh and saline water behaving as immiscible fluids, SWS 2012b).
Hydraulic parameters (hydraulic conductivity, specific yield and specific storage) of the Gunnedah and Narrabri Formations of the	Flow and transport simulations only consider Gunnedah and Narrabri Formations, for which non-uniform hydrogeological parameters exist in

Model assumptions	Relevance for current assessments
Upper Namoi Alluvium (Table 4.6) are based on calibrated values that are variable between, but uniform within, zones as used in the Upper Namoi Groundwater Flow Model (McNeilage 2006). For all other model layers, initial hydraulic parameters are assigned uniformly (homogeneous) but treated as variable during calibration.	the model.
Stream bed elevations are from the digital terrain model. Stream bed conductances are taken from the Upper Namoi groundwater model where possible. Conductances of additional reaches fall within the range of conductances in the Upper Namoi model dataset. Only these conductance values were adjusted during model calibration.	These are acceptable assumptions for generic calculations with assumptions that produce high end estimates. For the purpose of the assessment river bed hydraulic conductivities can be modified within reasonable bounds to quantify the sensitivity of the stream flows.
The geometry of the numerical layers is based on the geological model.	This is an acceptable starting assumption for the alluvial aquifer layers in developing the high-resolution solute transport models. After grid refinement several numerical layers will fit in each geological layer.
The Hunter-Mooki Fault System is assumed to be a no-flow boundary to the east of the groundwater model following an expectation of minimal groundwater flow across the fault.	The two areas selected for flow and transport modelling in the alluvial aquifers are sufficiently far from the Fault System for the no-flow boundary assumption to have no impact.

The NCM was reviewed for Stage 2 by Geoscience Australia (2011) (Table 4.2) and by members of the current project team for Phase 3 (Table 4.3) of model development. It is important to note the limitations identified in these reviews as they have relevance for the local models developed from the NCM. The major criticisms relevant to the shallow groundwater simulations were that it was not possible to assess whether the parameter values used in the numerical modelling were valid, and there should be improvements to the modelling of interactions between groundwater and surface water, especially for the gaining river sections.

Table 4.2 Model evaluation of Namoi Catchment Water Study - Phase 2 Report (additional comments in parentheses relate specifically to the current exposure Assessment)

Review comments confirming adequacy for intended purpose	Review comments indicating data and or model gaps
Data collation for the development of the conceptual geological model is adequate	It is not possible to assess if parameter values used for numerical modelling are valid
A good explanation of how the data were analysed is provided	Some discrepancies in geological data (but nothing critical for the purpose of shallow groundwater assessments)
A good analysis of data gaps for the conceptual geological model and proposed numerical model is provided	Lack of knowledge on aquifer connectivity (although critical in assessing the impact of coal seam gas extraction, it is not critical for

Review comments confirming adequacy for intended purpose	Review comments indicating data and or model gaps
	the purpose of transport calculations in shallow groundwater)
Model design and rationale are clearly discussed and are generally sound	Develop multiphase model in parallel to identify significance of a single-phase rather than a multiphase modelling approach (this is not relevant for shallow groundwater)

Several of the model limitations indicated in Table 4.2, Table 4.3 and Table 4.4 are not critical for transport calculations in shallow aquifers as they concern mainly deeper formations (e.g. connectivity between aquifers across aquitards). The need for a better model description of surface water to groundwater interaction is addressed in part in the current exposure assessment by means of using models with a much finer numerical grid which allows at least a higher spatial resolution in representing the geometry of the interface between the aquifer and the streams. The fact that the assessments will be generic rather than site-specific makes the model limitations even less critical (Table 4.4).

Table 4.3 Model evaluation of Namoi Catchment Water Study—Phase 3 Report (additional comments in parentheses relate to the current exposure assessment)

Review comments indicating model limitations	Critical for a high end exposure assessment in case of shallow groundwater?
Improve modelling of interactions between groundwater and surface water prior to commencing a transient simulation of the historic model	No, if discharge is not explicitly part of the transport pathway. Not critical for initial assessments of solute transport from a spill to shallow aquifer observation wells, i.e. not involving discharge to rivers
	Yes, if discharge to rivers is part of the transport pathway. Especially for the gaining river sections where the groundwater flux (and solute flux) into the river needs to be modelled realistically
Improve model calibration	No, for chosen sub-models covering the alluvial aquifers calibration is acceptable.
Undertake steady state calibration	Yes, transport calculations will be for steady state flows
Improve parameterisation of hard rock aquifers	No, not relevant for assessments for shallow alluvial groundwater

The need for a calibrated (and verified) groundwater model can be relaxed for a generic exposure assessment. A reasonable degree of calibration is sufficient to ensure that the simulated flows provide a reasonable description of the modelled system, albeit with some limitations. As the assessment becomes more site-specific at higher Tiers, the need for calibration increases. Thus, the requirement for improved model calibration, including steady state calibration (see Table 4.3), becomes important mainly for site-specific assessments. Note that the current version of the NCM was calibrated under transient or time-dependent groundwater flow conditions. The best performance was obtained for the alluvial aquifers with a coefficient of determination equal to 0.94 and a water balance error of 5 per cent (SWS 2012a). The comparison between time series of observed and simulated groundwater levels, or hydrograph matching, was particularly good in three of the zones that are also part of this study's two local models (see Figure 4.3). While such good model performance adds confidence to the assessment, the importance of calibration and validation should not be overestimated in a generic assessment where the key parameters for groundwater flow and solute transport will be perturbed over a fairly large range to provide results representative of a much larger area.

Table 4.4 Evaluation of model limitations for high end exposure assessments

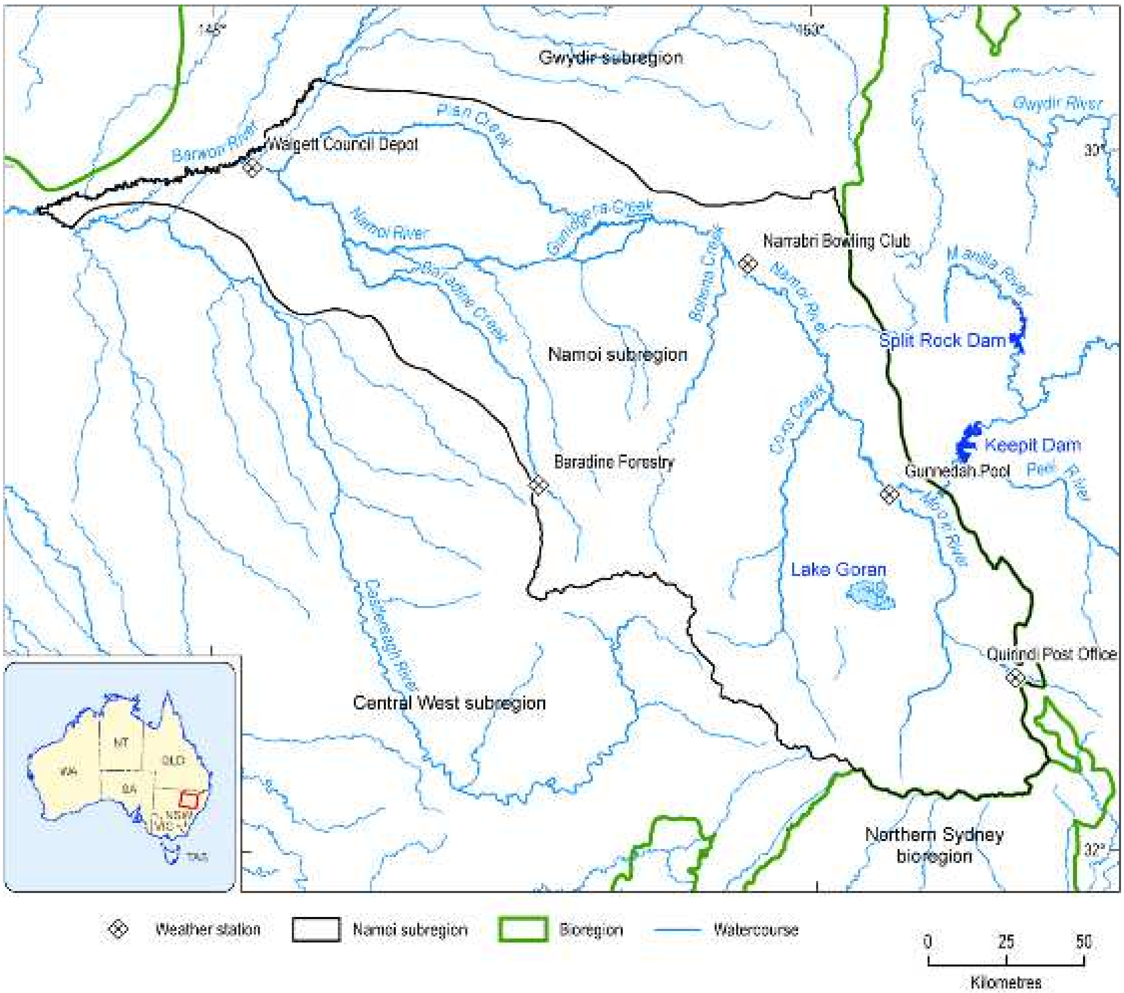
Model limitations	**Critical for a high end exposure assessment?**
Traceability: how the hydrogeological and hydrochemical datasets have been incorporated to inform the numerical modelling of the groundwater system	Yes. Traceability is critical for any assessment. At least for the shallow groundwater the starting conditions ('reference model') should be known including its underlying assumptions (even if very simplified).
Accuracy: lack of calibration against observed data to ensure the model provides a representative simulation of the natural system and processes.	No. There is no need for an accurate reproduction of the site-specific system and processes as the model will be set up to produce a range of outputs representing a broad range of groundwater flow conditions. That is, the perturbations will result in the calculated heads and velocities differing from the site-specific conditions anyway.
Adequate system representation: 'minor' faulting within the catchment cannot be captured by a regional scale model.	No. Transport calculations involve a very small computational domain incorporating local features rather than regional. While faults may have an impact on solute transport when deep groundwater (and deep contaminant sources) is involved, faults are generally less important for shallow groundwater and contaminant sources at the surface (in some cases they provide a barrier to flow).
Fit for purpose: the degree of connectivity between the alluvium and hard rock aquifers represents a significant data gap for this study at the present time.	No. As the focus in phase 1 is on shallow groundwater, there is less need for an accurate representation of such connectivity with deeper units. Unless faults are present, the very shallow groundwater is relatively insensitive to the way the deeper layers are connected.

Based on the above analysis, the NCM is "fit for purpose" and there is a high degree of confidence in using the NCM as a starting point for transport calculations in shallow groundwater of the Lower and Upper Namoi Alluvium in the Narrabri and Gunnedah Formations. However, to simulate deeper groundwater underlying the alluvium or shallow groundwater in non-alluvial layers outcropping at the surface, model improvements would be needed, or another model would need to be used.

4.3 Catchment characteristics

4.3.1 Geography

The Namoi catchment is in north-eastern New South Wales, and is based around the Namoi, Manilla and Peel rivers (Figure 4.2). It is bounded to the east by the Great Dividing Range, to the north by the Gwydir River catchment, to the south by the Macquarie-Castlereagh region and to the west by the Barwon-Darling region. The Namoi River and its main tributary, the Peel River, rise in the Great Dividing Range at elevations over 1 000 m, falling to 250 m where the two rivers meet near Gunnedah. The river then flows through sedimentary slopes (a midslope land unit fringing the Liverpool Plains, Duri Hills and East Pilliga Hills) to the open floodplains in the west. Nearly two-thirds of the region is comparatively flat[4]. The NCM covers an area of 30 380 km^2 and is enclosed within the boundaries of the Namoi catchment boundary.



[4] Namoi Catchment Authority website (www.namoi.cma.nsw.gov.au)

Source: Commonwealth of Australia (2014); Author, Welsh et al. (2014)

Figure 4.2 Namoi River with significant tributaries; only part of the catchment is enclosed by the subregion

The Namoi catchment covers an area of 41 856 km^2, corresponding to 4% of the area of the Murray-Darling Basin. Other major tributaries of the Namoi River include the Manilla and McDonald rivers, Coxs Creek, and the Mooki and Cockburn rivers, all of which join the Namoi upstream of Boggabri. The Namoi River then flows westerly across the western plains and joins the Barwon River near Walgett. Regulation in the catchment includes Keepit Dam (capacity 426 GL), Chaffey Dam (capacity around 63 GL), Split Rock Dam (capacity 397 GL) and a number of weirs.

4.3.2 Ecology

The Namoi catchment is an ecologically significant area because it includes:

- A wide range of aquatic habitats of ecological importance, including large areas of anabranch and billabong wetlands downstream of Narrabri (Figure 4.2).
- Endangered ecological communities in the vicinity of Lake Goran, which is listed in the Directory of Important Wetlands in Australia (Environment Australia 2001) and provides habitat for large numbers of waterbirds; and Gulligal Lagoon, which is important for native fish.
- Vulnerable, threatened, or endangered species[5], including the fish silver perch (*Bidyanus bidyanus*); the birds Australasian bittern (*Botaurus poicioptilus),* Australian bustard (*Ardeotis australis*), black-tailed godwit (*Limosa limosa*), and brolga (*Grus rubicunda*); and the turtle Bell's turtle (*Wollumbinia belli*).
- A variety of endangered flora including coolabah Bertrya (*Bertrya opponens*), river red gum (*Eucalyptus camaldulensis*) and river cooba (*Acacia stenophylla*); and six vegetation communities including Carbeen (*Corymbia tessellaris*), Open Forest, and bimble box (*Eucalyptus populnea*) woodland along the Namoi river.

The sole wetland of national importance in the Namoi region is Lake Goran (DIWA reference number NSW005). This lake is situated at the end of an internal drainage basin and does not connect to the Namoi River.

Another important ecological site is Gulligal Lagoon, near Gunnedah, which is a semi-permanent wetland that is connected to the Namoi River. The lagoon is filled during flood events and from surface runoff flows (Barma Water Resources et al. 2012), and provides important habitat for native fish species including the olive perchlet (*Ambassis agassizii*). The lagoon acts as a drought refuge in the mid-Namoi region and was restocked with breeding pairs of purple spotted gudgeon (*Mogurnda adspersa*) in late 2009 as part of the Namoi Demonstration Reach project.

The catchment has three topographic regions: the highlands and hills to the east of the Hunter-Mooki Fault, a flatter central region with extensive alluvial plains bounded by low hills, and floodplain areas to the west that are extremely flat (SWS 2011). The Namoi catchment is a westerly draining system with headwaters on the western flank of the Great Dividing Range and the Namoi River is the main drainage channel (SWS 2011), eventually draining into the Darling River.

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[5] New South Wales Government (2014b)

4.3.3 Climate

Total annual rainfall is highly variable throughout the catchment, with the topographically higher areas in the east receiving up to 1 300 mm, while the average in the lower elevation floodplains to the far west is only 480 mm (BOM 2011). From 1948 to 2010 the average annual rainfall recorded at Gunnedah Resource Centre (BOM station 55 024, elevation 307 m, latitude 31.03 °S, longitude 150.27 °E) was 638 mm/yr. Long term evaporation at the Gunnedah Resources Centre over the same time period was 1 596 mm/yr, or approximately 2.5 times higher than annual rainfall. The average annual rainfall at the Narrabri Bowling Club AWS is 643.2 mm, averaged from 130 years of rainfall data). The highest monthly rainfalls occur during January and February with the lowest rainfall generally experienced in April, August and September.

December, January and February are the warmest months with mean daily maximum temperatures at the Gunnedah Resources Centre of between 33.9°C and 35.3°C. June, July and August are the coolest months of the year on average with mean daily minimum temperatures between 3.4°C and 4.9°C.

4.3.4 Geology

The NCM model encompasses the entire Namoi catchment area (42 000 km^2) from ground surface to the top of the regional volcanic basement, a depth of -2 000 mAHD (SWS 2011). There are three main geological areas (east, central and west), and the eastern area of the catchment is separated from the central region by the Hunter-Mooki Fault (Figure 4.5). The New England Fold Belt deposits to the east have not been extensively explored for unconventional gas and since it was not possible to construct a detailed geological model for this area, it was excluded in the numerical groundwater model (SWS 2012a). The Gunnedah Basin is the central part of the catchment and is composed of sedimentary and volcanic strata of Permian and Triassic age (SWS 2012a). The geology of the central portion of the catchment is better understood than the east and west portions of the catchment. The Surat Basin in the western portion of the catchment is a sub-basin of the Great Artesian Basin. The data in this area are much sparser and there is less certainty regarding the geology (SWS 2012a). The strata are thought to dip toward the northwest in the centre of the Surat Basin. The Hunter-Mooki Fault trends north-northwesterly and is thought to cut through all of the Permian, Triassic and Jurassic strata, but not the uppermost alluvial surfaces (SWS 2012a).

In the NCM, the lower part of the stratigraphy consists of Upper and Lower Permian coal bearing layers (Black Jack and Maules Creek Formations), separated by the Mid Permian marine sediments of the Porcupine and Watermark Formations, and underlain by the basal Lower Permian Goonbri and Leard Formations (Tadros 1993; SWS 2012a; Figure 4.6 and Figure 4.7). The overlying Triassic units are classed as mainly minor aquifers consisting of the Digby, Napperby and Deriah Formations. The Triassic units are overlain by Jurassic units consisting of the Garrawilla Volcanics, a minor aquifer, and mainly sandstone aquifers of the Purlawaugh Formation and Pilliga Sandstone (Figure 4.6). The material overlying the Pilliga Sandstone could not be separated into constituent members and was therefore grouped into a single model layer referred to as the Great Artesian Basin, an aquifer consisting of a mixture of sandstone, siltstone, mudstone and minor thin coal seams (SWS 2011;Table 4.5).

Closer to the land surface, the following three layers are relevant in the current study where contamination of shallow groundwater is of concern. Layer 3 in the NCM is a Quaternary weathered zone / fractured rock aquifer that extends east of the Hunter-Mooki fault system. This is overlain by the Narrabri Formation and Gunnedah Formation. These have been grouped in the numerical model as Layers 1 and 2 respectively, and are commonly referred to as the shallow alluvial aquifers that overlie the hard rock aquifers (clastic sedimentary rocks and volcanics).

The conceptualisation in the NCM is consistent with the study by CSIRO (2007) which indicates that the Namoi groundwater system is recharged through:

- infiltration of the stream water in the Namoi River via river bed and bank infiltration particularly during periods of high flow or extended periods of low to medium flow
- deep drainage of rainfall, overland flow, natural ponding and applied irrigation water through the alluvial surfaces
- groundwater inflows from connected alluvial aquifers associated with tributary systems.

In conceptual models, the Namoi catchment is divided into the Lower and Upper Namoi. The alluvial sediments of the Upper Namoi are usually subdivided into two formations (Williams 1986; SWS 2011). The uppermost formation is the Pleistocene to Quaternary Narrabri Formation (approximately 30 m in average thickness) which consists predominantly of clays with minor sand and gravel beds (Williams1986). These lens-shaped deposits provide generally low yielding aquifers of low to medium salinity (Williams 1986). Underlying the Narrabri Formation is the Pliocene to early Pleistocene Gunnedah Formation (up to 115 m in thickness), which consists predominantly of gravel and sand with minor clay beds and is the principal aquifer used for irrigation. The gravels and sands are often high yielding, good water quality aquifers and the most productive aquifers of the Gunnedah Formation are within paleochannels which contain coarser sediments deposited by powerful streams (Broughton 1994; McNeilage 2006). The maximum combined depth of the two formations is unlikely to exceed 170 m. The two formations have been found to have good hydraulic connectivity (McNeilage 2006). Hydrogeological parameters (horizontal and vertical hydraulic conductivity, specific yield and specific storage) are listed in Table 4.5 and were collated from the literature and used as starting values during calibration of the NCM (SWS 2012a).

The Lower Namoi alluvium has two separate layers: the Gunnedah and Cubbaroo Formations and reaches a maximum thickness of 120 m. Since the Narrabri Formation does not occur in the Lower Namoi, the uppermost aquifer in this subregion is part of the Gunnedah formation. In the Lower Namoi the alluvial deposits of the Cubbaroo Formation underlie those of the Gunnedah Formation. The Cubbaroo Formation consists of sand and gravel with interbedded brown to yellow and grey clay of middle to late Miocene age (Williams 1986). Cubbaroo Formation sediments infill the pre-tertiary channels of the Lower Namoi (Williams 1986).

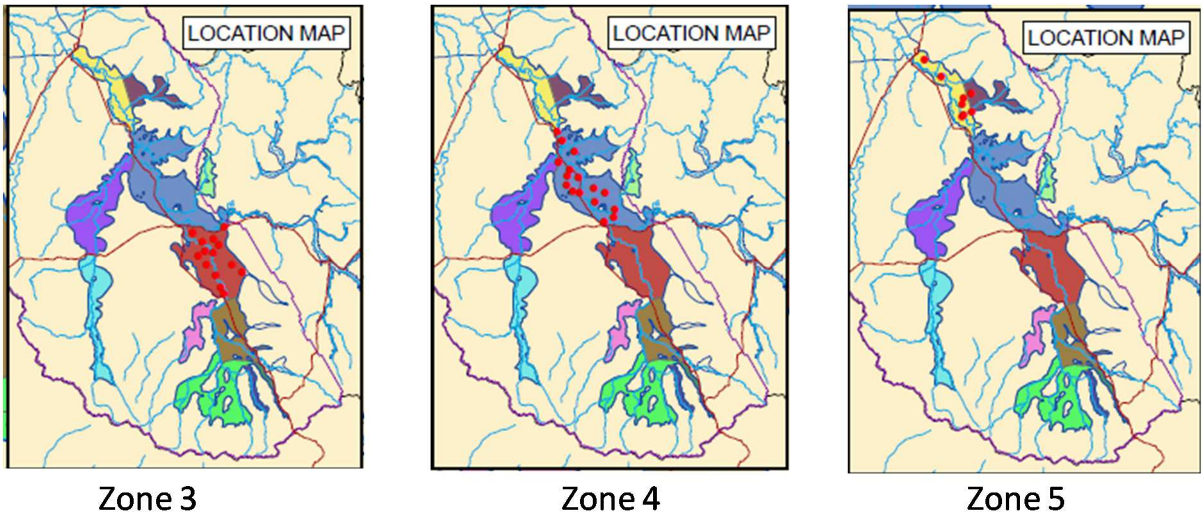
The basement for the alluvium in the Namoi catchment consists of clastic sedimentary rocks of the Great Artesian Basin or volcanic rocks of Miocene age (Radke et al. 2012).

There is a long history of groundwater model development of the alluvial systems, which SWS referred to in calibrating hydraulic parameters in the NCM (SWS 2012b). The shallow alluvial aquifers (Layers 1 and 2) were modelled previously by McNeilage (2006) and reported in SWS (2011) as the 'Upper Namoi Model'; the hydraulic parameters K_H (horizontal conductivity), K_V (vertical conductivity), S_y (specific yield), and S_s (specific storage) for the Narrabri and Gunnedah Formations (Table 4.6) are well-calibrated in this previous work (Figure 4.3). Although these hydraulic parameters are not used in the current model, they are given for the purpose of traceability (they are the basis for additional calibrations that have not been reported previously but are now covered in Appendix A). The Upper Namoi model parameters are given in Table 4.7. Previous groundwater modelling was also conducted for the Lower Namoi groundwater management area, referred to as the Lower Namoi Alluvium groundwater models by Merrick (2001). SWS (2011) acknowledges that there is very little specific data publically available for the 2001 model; the data they were given are listed as Lower Namoi model values assigned to the Gunnedah Formation (Table 4.6).

Table 4.5 Hydrogeological properties collated from the literature and used as starting values for calibration of the Namoi Catchment Model

Geological units	Hydrogeological significance	Horizontal hydraulic conductivity, K_H (m/d)	Vertical hydraulic conductivity, K_V (m/d)	Specific yield, S_y	Specific storage, S_S (1/L)
Narrabri Formation	Significant Aquifer	0.1–30[a] (6.3)[a]	0.000001.7 to 0.037[a] (0.0003[a])	0.005 to 0.1[a]	0.000005[b]
Gunnedah formation	Significant Aquifer	0.05–30[a] (7.1[a])	3.2 to 7.2[d]	0.15[d]	0.000001 to 0.0005[a]
Lower Namoi/Weathered Horizon	Significant Aquifer	0.0009 to 8.6[f]	0.009 to 0.9[f]	0.15[d]	0.000001 to 0.0005[a]
Fractured rock horizon	Aquifer	0.01 to10[f]	0.001 to 0.1[f]	0.01[f]	0.00001[f]
Great Artesian Basin	Aquifer	0.004 to 0.265[b]	0.000015 to 0.0002[b]	0.1[e]	0.0001 to 0.00001[e]
Pilliga Sandstone	Aquifer	0.004 to 0.265[b]	0.000015 to 0.0002[b]	0.1[b]	0.000005[b]
Purlawaugh Formation	Aquifer	0.004 to 0.02[b]	0.000015 to 0.001[b]	0.001[b]	0.000005[b]
Garrawilla Volcanics	Minor Aquifer	0.001 to 0.04[b]	0.000006 to 0.001[b]	0.002[b]	0.000005[b]
Napperby and Deriah Formation	Minor Aquifer	0.001 to 0.04[b]	0.000006[b] to 0.71[d]	0.1[d]	0.0001[d]
Digby Formation	Minor Aquifer	0.9 to 1.5[d]	0.62 to 0.71[d]	0.1[d]	0.0001[d]
Upper Black Jack	Aquitard	0.0003 to 1.1[d]	0.19 to 0.59[d]	0.1[c]	0.00001[d]
Hoskissons seam	Aquifer	0.13 to 3.3[c]	0.00022 to 0.002[c]	0.2[c]	0.0001[c]
Middle Black Jack	Aquitard	0.0015 to 0.047[d]	0.005 to 0.4[d]	0.1[d]	0.0001[d]
Melvilles seam	Aquifer	0.02[g]	0.005 to 0.4[g]	0.1[g]	0.0001[g]
Lower Black Jack	Aquitard	0.0015 to 0.047[d]	0.005 to 0.4[d]	0.1[d]	0.0001[d]
Watermark and Porcupine Formation	Aquitard	0.0009 to 0.00014[f]	0.00009 to 0.0014[f]	0.01	0.00001[d]
Maules Creek Formation	Aquifer	0.13 to 3.3[c]	0.00022 to 0.002[c]	0.1[c]	0.0001[c]
Leard formation	Aquitard	0.009 to 0.25[f]	0.0009 to 0.025[f]	0.01[f]	0.00001[f]

Model developed by Schlumberger Water Services Ltd (SWS 2012a). Data sources:
a = NSW Office of Water (2010), b = Aquaterra (2009), c = Golder Associates (2008), d = Golder Associates (2010), e = GABCC (2010), f = Freeze and Cherry (1979), g = Geoterra (2008).



Source: SWS (2012a). Red dots are monitoring wells used for model calibration.

Figure 4.3 Zones within the Upper Namoi Alluvium model where groundwater level matching was good (water balance error at most 5% and coefficient of determination R^2 = 0.94)

Table 4.6 Calibrated model parameters (for Upper Namoi Model see Table 4.7)

Geological units	**MODFLOW model Layer**	K_H/K_V **(m/d)**	S_y/S_s **(%;1/m)**
Narrabri Formation	1	As Upper Namoi Model	As Upper Namoi Model
Gunnedah Formation	2	As Upper Namoi Model Lower Namoi 5/0.5	As Upper Namoi Model Lower Namoi 10/0.001
Weathered zone	3	As layers below	As layers below
Fractured rock aquifer	4	0.1/0.01	1/1x10^{-5}
Great Artesian Basin	5	0.1 /0.0001	10/1x10^{-5}
Undefined	5	0.01/0.0001	1/5x10^{-6}
Pilliga Sandstone	6	0.05/0.0001	10/5x10^{-6}
Purlawaugh Formation	7	0.01/0.0001	1/5x10^{-6}
Garrawilla Volcanics	8	0.01/0.00001	1/5x10^{-6}
Napperby and Deriah Formation	9	0.02/0.001	10/1x10^{-6}
Digby Formation	10	0.02/0.001	10/1x10^{-6}
Upper Black Jack Formation	11	0.01/0.00001	10/1x10^{-6}
Hoskissons Seam	12	0.01/0.00001	15/5x10^{-6}
Middle Black Jack Formation	13	0.01/0.00001	10/1x10^{-6}
Melville Seam	14	0.01/0.00001	15/5x10^{-6}

Geological units	MODFLOW model Layer	K_H/K_V (m/d)	S_y/S_s (%;1/m)
Lower Black Jack Formation	15	0.01/0.00001	$10/1x10^{-6}$
Watermark and Porcupine Formation	16	0.01/0.001	$1/1x10^{-6}$
Maules Creek Upper Buffer	17	0.01/0.0001	$2.5/5x10^{-6}$
Maules Creek Formation	18	0.01/0.0001	$2.5/5x10^{-6}$
Maules Creek Lower Buffer	19	0.01/0.0001	$2.5/5x10^{-6}$
Goonbri and Leard Formation	20	0.01/0.001	$1/1x10^{-6}$
Willow Tree Formation	5	0.01/0.001	$1/1x10^{-4}$
Boggabri Volcanics	5	0.001/0.0001	$1/1x10^{-6}$

Source: SWS (2012a)

Solute transport simulations require knowledge about the (effective) porosity parameter, η_e. Based on this parameter, the solute pore-water velocity *v* is calculated from the groundwater flow velocity *q*, according to the formula:

$$v = \frac{q}{\eta_e} \qquad \text{[Equation 2]}$$

Where:

v = solute pore-water velocity

q = groundwater flow velocity

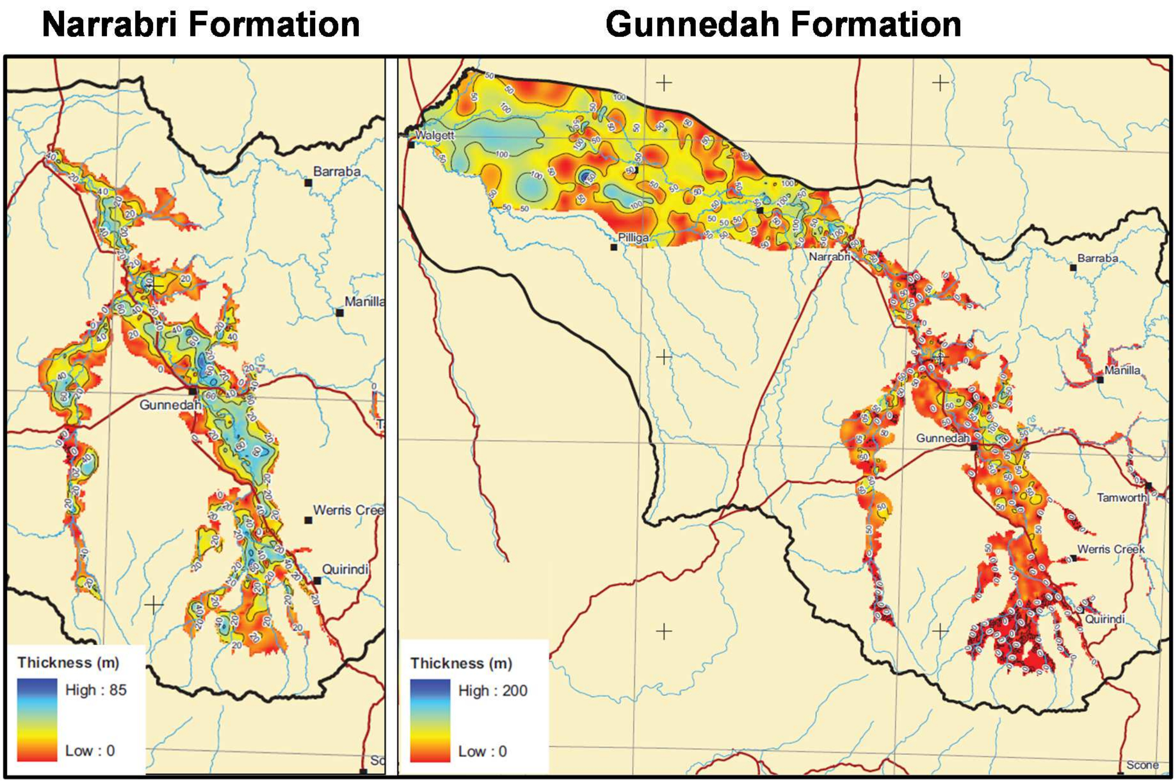
η_e = effective porosity

In calculating *v*, the effective porosity η_e rather than the total porosity η is used because not all pore spaces contribute to solute transport. Differences between total and effective porosity are small for gravel and sand. For such materials, putting effective porosity equal to total porosity is unlikely to introduce large errors. For loam and clay material, differences between η_e and η are larger (de Marsily 1986), and η_e needs to be determined separately.

Reported porosity[6] values of the alluvial formations vary in the broad range from 0.15 to 0.39. Average total porosity[7] of the Maules Creek[8] alluvium (highly heterogeneous sediments composed of medium to heavy clays, sands, gravels and boulders), obtained through oven drying and weighing in the laboratory was between 0.31 and 0.39 with a mean of 0.32 (Rau et al. 2010). Timms and Ackworth (2005) assumed a porosity of 0.15 for the shallow confined aquifer formation at Liverpool plains (poorly sorted gravels underlying silt-clay deposits). This range in porosity values reflects the natural variability in the alluvial

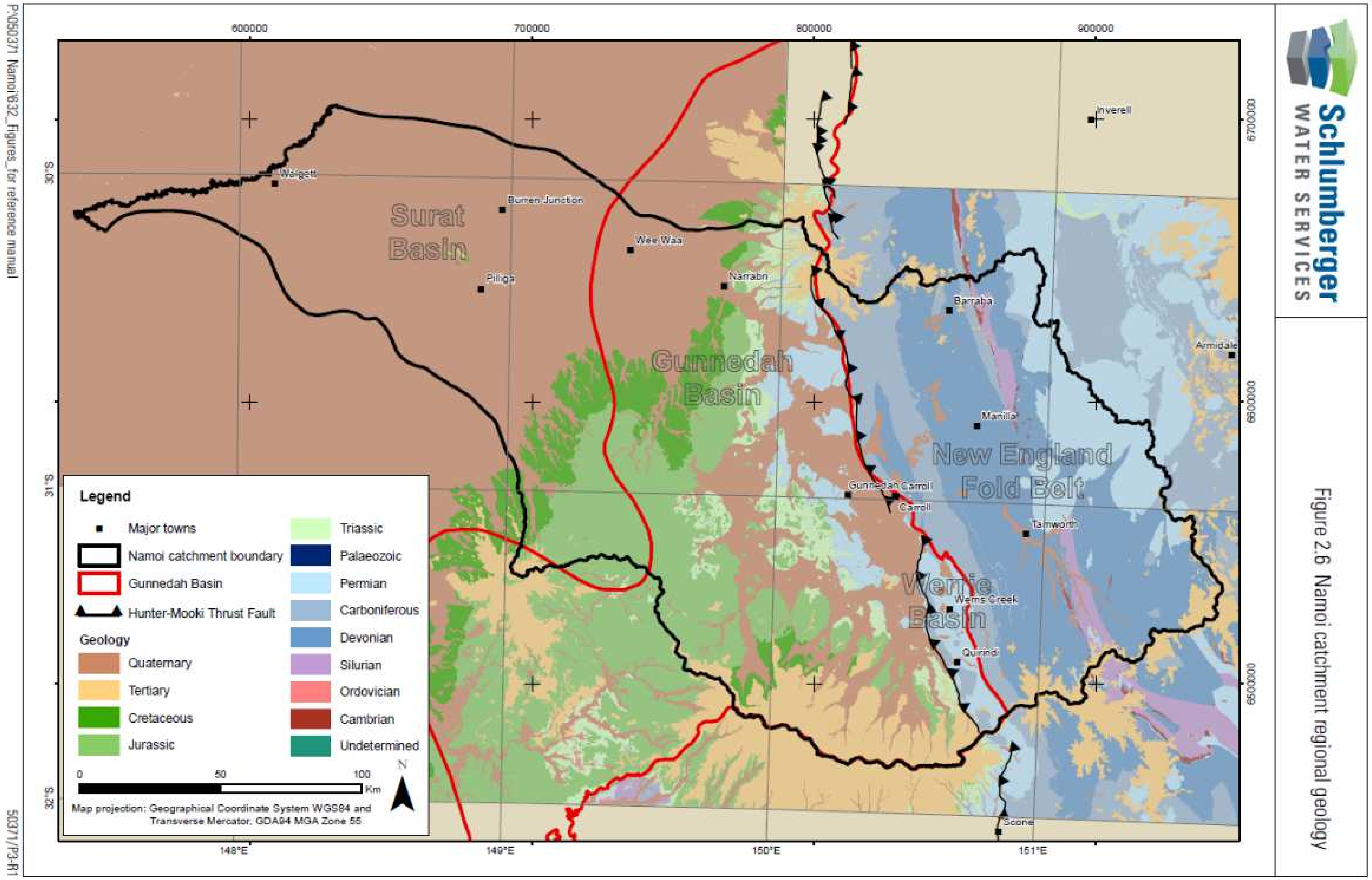
[6] Total porosity is assumed
[7] Assuming a solid density of 2.65 g/cm^3
[8] Tributary of the Namoi River between Narrabri and Boggabri

sediments; a similar range will be used in the exposure assessment calculations (Mallants et al. 2017b).



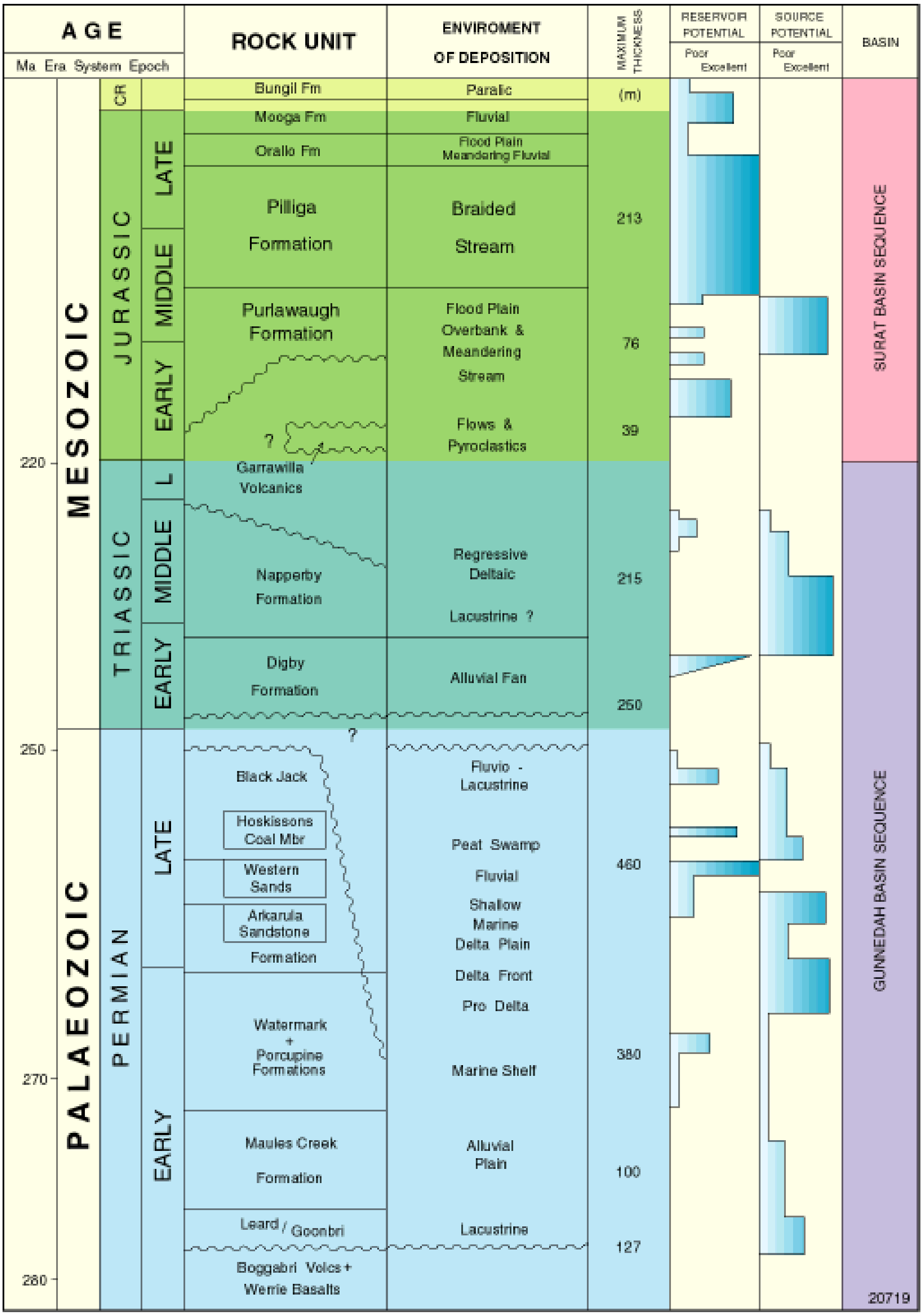
Source: SWS (2011)

Figure 4.4 Location and thickness of the Narrabri Formation and underlying Gunnedah Formation



Source: SWS (2012a)

Figure 4.5 Namoi catchment regional geology showing the Hunter-Mooki Fault and the main geological areas of the catchment



Source: NSW Department of Trade and Investment (2013). Note: The column 'Reservoir Potential' indicates the potential of the rocks of the formation to store hydrocarbons. The column 'Source Potential' indicates the potential of the rocks of the formation to produce hydrocarbons.

Figure 4.6 Stratigraphic column for the Gunnedah Basin and the overlying Surat Basin.

<table>
<tr><th>Period</th><th colspan="4">Litho-stratigraphy</th><th>Main rock types</th></tr>
<tr><td rowspan="2">Quaternary</td><td rowspan="2">Unconsolidated sediments</td><td colspan="3">Narrabri Formation</td><td>Clays, minor sands and gravel beds</td></tr>
<tr><td colspan="3">Gunnedah Formation</td><td>Gravel and sand with minor clay beds</td></tr>
<tr><td rowspan="3">Triassic</td><td rowspan="16">Gunnedah Basin Sequence</td><td colspan="3">Napperby Formation</td><td>Interbedded fine sandstone & siltstone</td></tr>
<tr><td rowspan="2">Digby Formation</td><td colspan="2">Ulinda Sandstone</td><td>Quartz sandstone</td></tr>
<tr><td colspan="2">Bomera Conglomerate</td><td>Conglomerate</td></tr>
<tr><td rowspan="11">Late Permian</td><td rowspan="11">Black Jack Group</td><td rowspan="2">Nea Subgroup</td><td>Trinkey Formation</td><td>Coal measures – siltstone, fine sandstone, tuffs, stony coal</td></tr>
<tr><td>Wallala Formation</td><td>Conglomerate, sandstone, siltstone, minor coal bands</td></tr>
<tr><td rowspan="5">Coogal Subgroup</td><td>Breeza Coal</td><td>Coal & claystone</td></tr>
<tr><td>Clare Sandstone</td><td>Medium to coarse-grained quartzose sandstone; quartzose conglomerate</td></tr>
<tr><td>Howes Hill Coal</td><td>Coal</td></tr>
<tr><td>Benelabri Formation</td><td>Claystone, siltstone & sandstone; fining up cycles; more sandy towards top of unit</td></tr>
<tr><td>Hoskissons Coal</td><td>Coal, minor claystone bands</td></tr>
<tr><td rowspan="4">Brothers Subgroup</td><td>Brigalow Formation</td><td>Fining-up sequence of medium to coarse-grained quartzose sandstone and siltstone</td></tr>
<tr><td>Arkarula Formation</td><td>Sandstone & siltstone; burrowed & bioturbated</td></tr>
<tr><td>Melvilles Coal</td><td>Coal</td></tr>
<tr><td>Pamboola Formation</td><td>Sandstone, siltstone, minor claystone & coal</td></tr>
<tr><td rowspan="2">Mid Permian</td><td rowspan="2">Millie Group</td><td colspan="2">Watermark Formation</td><td>Marine – sandy siltstone/claystone, silt/sand laminite, sandstone</td></tr>
<tr><td colspan="2">Porcupine Formation</td><td>Marine – diamictite, sandy-mudstone</td></tr>
</table>

Source: Golder Associates (2010). Note: aquitards are shaded light brown, potential or poor aquifers are shaded light blue. Significant aquifers are shaded darker blue.

Figure 4.7 Summary stratigraphic table for the Gunnedah and overlying Surat Basins

Table 4.7 Calibrated aquifer parameters for Layers 1 and 2 for the Upper Namoi model. Vertical hydraulic conductivity is used to calculate interlayer leakage.

Model area	**Horizontal hydraulic conductivity (m/d)**		**Interlayer leakage (1/d)**	**Specific yield (-)**	**Specific storage (1/m)**
	Layer 1	***Layer 2***	***Layer 1/2***	***Layer 1***	***Layer 2***
Minimum	0.1	0.05	1.7×10^{-6}	0.005	1.0×10^{-7}
Maximum	30	30	3.7×10^{-2}	0.1	5.0×10^{-4}
Mean	6.3	7.1	3.0×10^{-4}	0.04	1.6×10^{-4}
Median	5.0	5.0	9.5×10^{-5}	0.03	1.0×10^{-4}
Std deviation	6.1	6.1	1.3×10^{-3}	0.027	1.7×10^{-4}

Source: SWS (2011) and from McNeilage (2006)

4.4 Conceptual exposure pathway models and risk simulators

The next section describes the conceptual exposure pathway models and a set of risk simulator modelling tools that are being developed to predict environmental concentrations in soil and shallow groundwater from surface handling of drilling and hydraulic fracturing chemicals and produced waters (site spills, overflows, runoff, and leaks from surface ponds). Using such modelling tools, concentrations, distributions and travel times for environmental contaminants will be determined for specific high end exposure scenarios.

Exposure assessments for humans were conducted by NICNAS, while the Chemical and Biotechnology Assessment Section (CBAS) conducted exposure assessments for the environment. The exposure assessment for human health required predicted concentrations in relevant receiving environments such as shallow groundwater and surface waters (rivers, wetlands, and springs) that receive groundwater through recharge processes.

5 Conceptual model for the soil-groundwater pathway

5.1 Models for source-pathway-receptor analysis

An assessment of the fate of solutes potentially leaking from surface sources to soil and groundwater and subsequent interactions with receiving environments, requires consideration of a chain of components of the landscape that are part of the soil-groundwater pathway. A simplified schematic of the pathway components and the computational endpoints for each component is shown in Figure 5.1. The four components considered in our exposure assessment are:

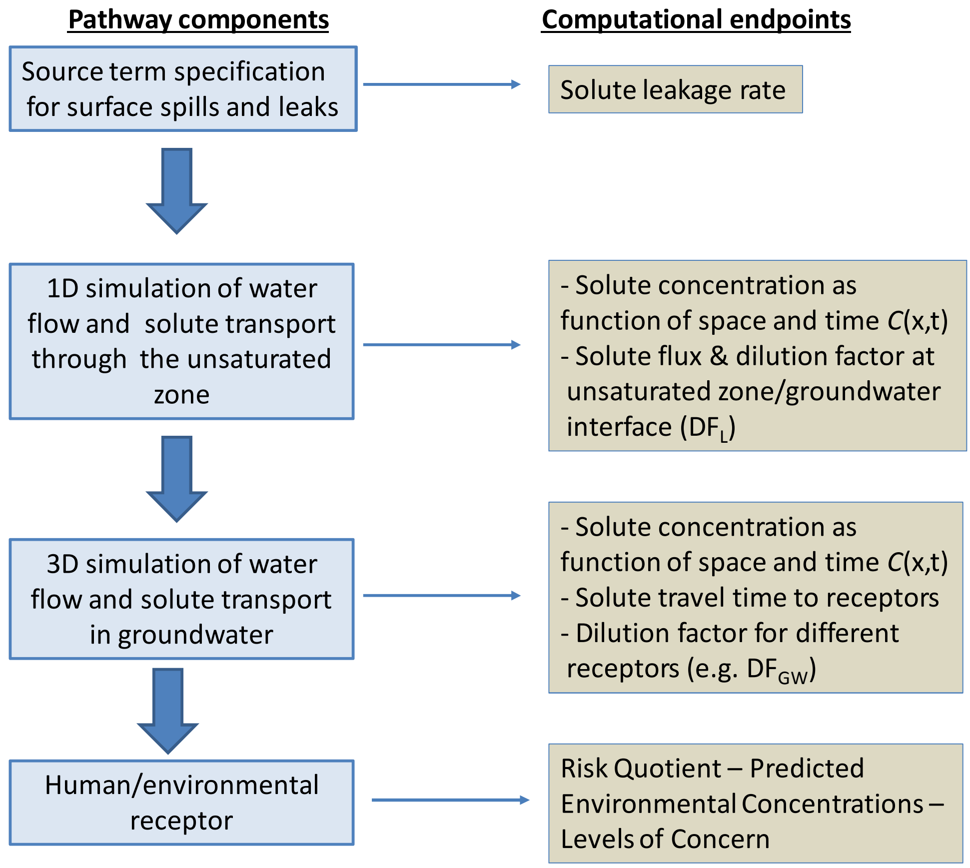
- specific source term for surface spills and leaks (resulting in a solute leak rate)
- simulation of water flow and solute transport through the unsaturated zone (resulting in solute concentrations within the soil profile and a dilution factor at the interface with the groundwatertable)
- simulation of water flow and solute transport in groundwater accounting for solute release into three receiving environments of wells, streams, and wetlands (resulting in dilution factors for each of such receiving environments)
- specific human and environmental receptors.

For each component, there is a set of computational endpoints that allows simulation results (e.g. solute concentration, dilution factors) to be used in other calculations, such as for response modelling.

Simulation of solute leaching by means of these four assessment components (source, soil pathway, groundwater pathway, and receptors) considers three source type scenarios (point, line, area source) and a range of solute volumes/leak durations to cover a plausible range of leak incidents at the surface of the production site. Details of the scenario parameters are provided in Table 3.3. At this phase of the exposure assessment (i.e. Tier 1), calculations will use hypothetical concentrations for a hypothetical solute (i.e. unit solute concentration of 1 mg/L). The hypothetical solute is assumed to behave as an ideal tracer in soil and groundwater (i.e. no interaction with the sediment particles, no degradation or other biogeochemical reactions, commensurate with the assumptions for a simplified model at Tier 1). This is a sufficient condition to derive dilution factors, travel times from source to receiving environment, and other computational endpoints. If computational endpoints such as solute fluxes or concentrations are required for specific chemicals, the results obtained for the hypothetical solutes can be readily rescaled to provide results for specific chemicals.

Solute transport through the unsaturated zone will provide estimates of chemical concentrations at any depth in this zone, including at the bottom, which corresponds to the groundwatertable. It is convenient to define the reduction in concentration (dilution) at the groundwatertable that has occurred from the solute travelling through the entire unsaturated zone. Likewise, a reduction in concentration can be defined as solutes travel in groundwater from their source (i.e. the interface with the unsaturated zone) towards a well (or any other receiving environment). For example, US EPA (1996) defined a Dilution Attenuation Factor (DAF) to account for dilution and attenuation as a result of processes such as sorption and biodegradation. The DAF is calculated as the ratio of original source concentration to the receiving environment concentration. The lowest possible value of DAF is therefore 1. When

DAF = 1 there is no dilution or attenuation at all; the concentration at the point of discharge to the receiving environment is the same as the source concentration. High DAF values on the other hand correspond to a high degree of dilution and attenuation. The term dilution factor (DF) is more appropriate when sorption and biodegradation processes are not accounted for (e.g. in a high end assessment such as the current exposure assessment).



Note. Each component provides a set of computational endpoints. For derivation of dilution factors DF_L and DF_{GW} see main text.

Figure 5.1 Components of the soil-groundwater pathway used to assess solute migration from surface storage systems and land surface spills via soil and groundwater pathways

Dilution occurs both in the unsaturated zone and in groundwater. A dilution factor is defined for the unsaturated zone (DF_L) to be the ratio of contaminant concentration in fluid leaked at the surface (C_{HF}) to the maximum contaminant concentration at the bottom of the unsaturated zone, i.e. at the watertable (C_{WT}) (Figure 5.2). The calculation of DF_L typically involves a one-dimensional solute transport model for the unsaturated zone; details of such models are provided in Section 5.2. The dilution factor for groundwater (DF_{GW}) is calculated as the ratio of the maximum contaminant concentration at the bottom of the unsaturated zone (C_{WT}) to the maximum concentration at a receiving well (C_{WELL}). The combined dilution in the unsaturated zone and groundwater (DF) is defined as:

$$DF = DF_L \times DF_{GW} \qquad \text{[Equation 3]}$$

Where:

DF = Dilution Factor (combined dilution in the unsaturated zone and groundwater)

DF_L = dilution factor for the unsaturated zone

DF_{GW} = dilution factor for groundwater

DF depends on a number of parameters such as the aquifer hydraulic conductivity, hydraulic gradient, infiltration rate, mixing zone depth, and source length parallel to groundwater flow (US EPA 1996).

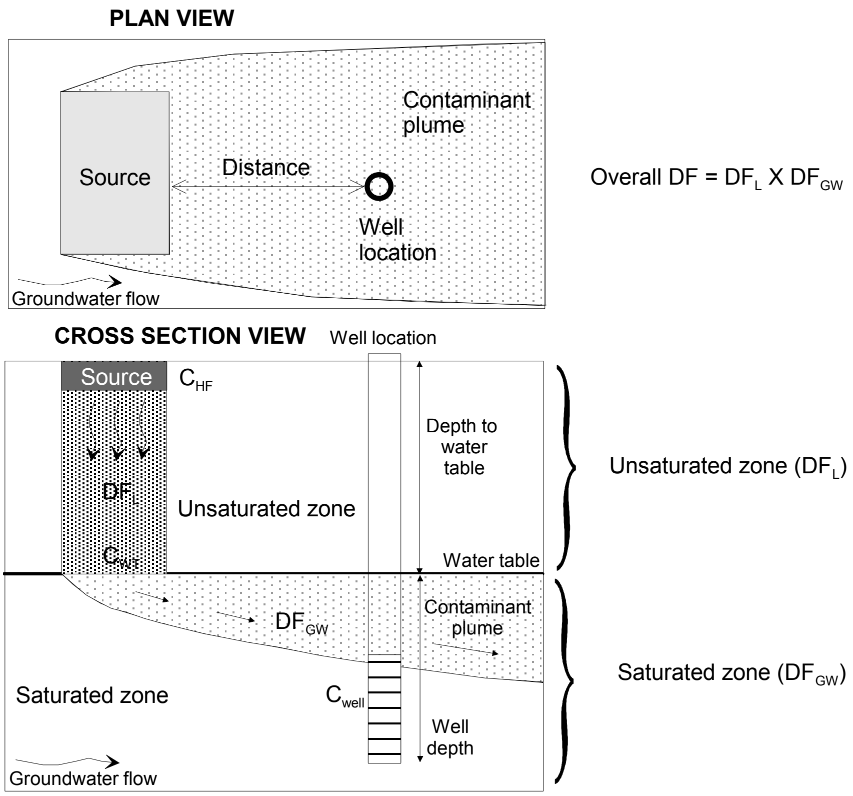
Once the dilution factors for the various receiving environments have been defined (a calculation that has to be done only once for a given source-pathway-receptor combination) the concentration at the watertable ($C_{COC,\ WT}$) or at the well ($C_{COC,\ GW}$) for any particular concentration of a specific chemical of concern (COPC – chemicals meeting several criteria were considered as potentially of concern, see NICNAS 2017b) in the surface source can be calculated using the following equations:

$$C_{COC,WT} = {C_{COC,HF}}/{DL_L} \quad \text{[Equation 4]}$$

$$C_{COC,GW} = {C_{COC,WT}}/{DF_{GW}} = {C_{COC,HF}}/{(DF_{GW} \times DF_L)} \quad \text{[Equation 5]}$$

A similar reasoning can be developed for the concentration in other receiving environments. For the dilution factors (and other computational endpoints) to be broadly applicable – that is, covering a sufficiently broad range of soil and groundwater flow conditions – multiple calculations of dilution factors will be undertaken with different soil and groundwater parameters that govern solute migration. The approach taken here is discussed in Section 5.3.

The single most important principle for long-term management of risks associated with hydraulic fracturing is to apply best-available-practices. This includes risk avoidance, risk minimisation and management, containment of chemicals, fluids, and treatment/containment and safe disposal of associated waste products. This is commensurate with the general principle that pollution prevention is preferred in limiting damage to humans and the environment. However, in case a spill or leak does occur, natural attenuation processes such as dilution and adsorption will reduce concentrations and thus reduce the risk. Although the above assessment approach is presented as dilution-based, at least from a mathematical point of view, the adopted source-pathway-receptor models apply basic physical principles of mass transport based on flowing water (advection) and mixing due to variations in flow velocities (dispersion) (Freeze and Cherry 1979; Mallants et al. 2000). These are natural processes that will occur in reality and that are the basis for a gradual decrease in concentration as distances from the chemical source increase. The assessments consider the following key receiving environments: soil and its ecosystems (mainly plants), groundwater, groundwater wells, streams, wetlands and springs (for a summary see Table 2.1). Typical computational endpoints for each of these receiving environments are also provided in Table 2.1.



Source: US EPA (1996)

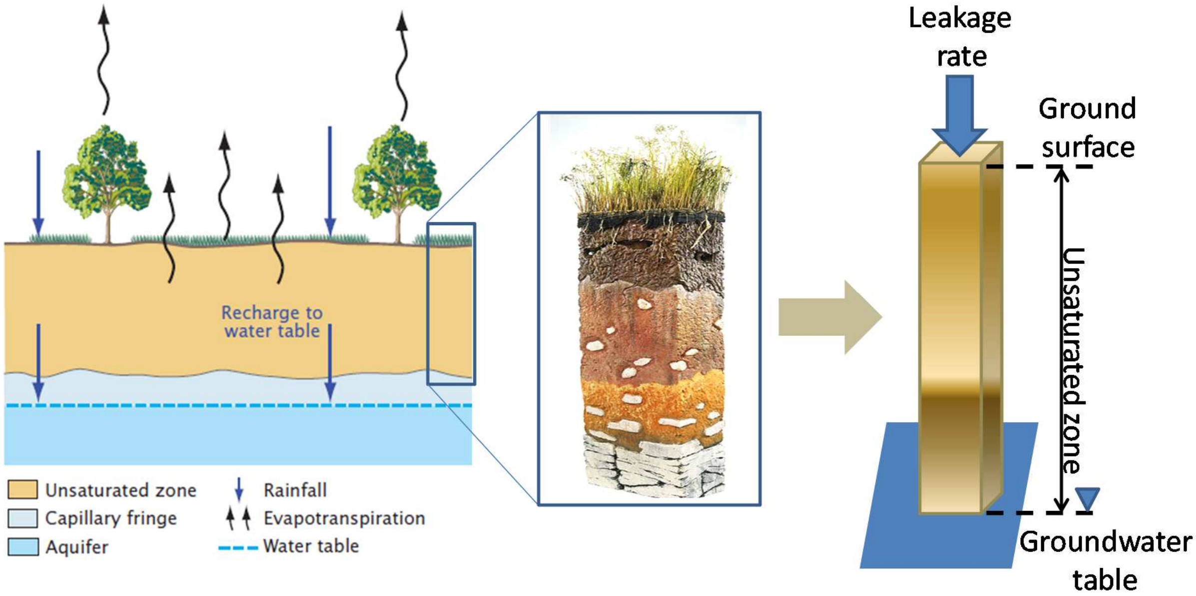
Figure 5.2 Dilution factors for unsaturated and saturated zone for soil to groundwater pathway.

5.2 Soil pathway

5.2.1 Simplifying assumptions

Water flow and contaminant transport from leaking sources to groundwater will be simulated through one-dimensional columns (Figure 5.3). A detailed discussion of the soil pathway was provided in Mallants et al. (2017a). For a realistic exposure assessment, models for impact assessment should be chosen on their ability to include all hydrological, chemical, and biological processes relevant to water flow and contaminant migration in soil (for a comprehensive review, see Mallants et al. 2011). However, because this project is a Tier 1 process only, the objective is to conduct a realistic high end estimate assessment; hence solute transport will be simplified to non-reactive transport.

Chemical interactions between contaminants and the soil minerals and biogeochemical transformations may be invoked in later phases if higher tier risk assessments are needed to quantify impacts on human health and the ecosystem (i.e. if the lower tiers indicate non-negligible impact). A summary of simplifying assumptions is provided in Table 5.1. Higher tier assessments using more realistic assumptions are typically undertaken if it is demonstrated at Tier 1 that the impact exceeds regulatory criteria or other levels of concern. The health risk assessment was explicitly a Tier 1 process only (NICNAS 2017d), as was this study. The environment risk assessment used a three-tiered process and did not draw on the shallow groundwater modelling (DoEE 2017c).



Source: CSIRO (2011) (left image); http://pixgood.com/soil-layers-diagram.html (middle image).

Figure 5.3 Conceptual diagram of water fluxes beneath the land surface to the watertable (left). Unsaturated zone profile (middle). Conceptual representation of the unsaturated zone as a soil column (right).

Table 5.1 Model simplifications imposed for Tier 1 assessments

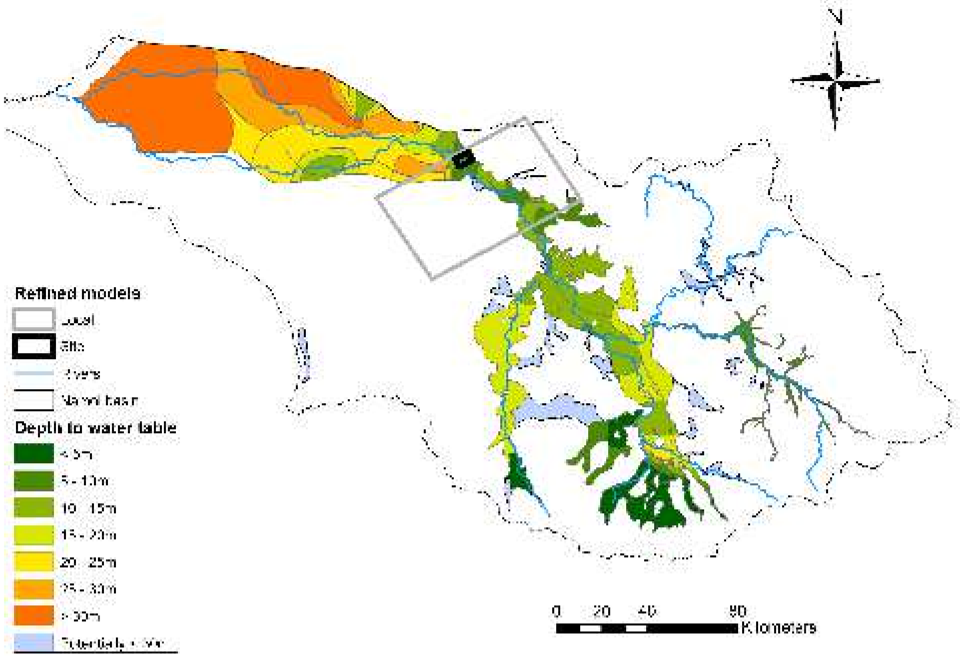
	Model simplifications	**Model modifications for Tier 2 assessments**
Processes	See Table 5.2 for an overview of processes	A summary of processes relevant for Tier 2 is available from Mallants et al. (2017a)
Parameters	Soil parameters relevant for water flow (hydraulic properties and plant parameters) have been simplified and represented by a spatially uniform recharge and a generic set of hydraulic properties. Soils in the catchment are represented by two contrasting materials (sand and loam) with a spatially uniform recharge value. This results in two different steady state water content profiles and hence two different chemical velocities. Soil layering has not been considered.	Explicit consideration of soil water balance calculations to determine recharge (different vegetation types accounted for). Soil map information used to generate soil hydraulic properties. Soil layering and deeper stratigraphy of the unsaturated zone included.
Boundary conditions	At the top of the unsaturated zone infiltration is taken as constant and spatially uniform. Infiltration is assumed equal to recharge (recharge occurs at the bottom of the unsaturated zone); this is justified because no losses due to evapotranspiration are simulated and steady	Time dependent recharge is calculated; recharge is spatially variable and is dependent on soil type and vegetation.

	Model simplifications	Model modifications for Tier 2 assessments
	state flow is assumed (i.e. in any year the amount of water entering the unsaturated zone at the top and leaving it at the bottom is identical). At the bottom of the unsaturated zone a stable groundwatertable is considered.	

5.2.2 Domain geometry

The use of a one-dimensional rather than a two or even three-dimensional water flow and solute transport model to simulate solute migration from the land surface to the groundwatertable is justified because flow in the unsaturated zone generally occurs in the vertical direction. Exceptions to this were discussed in Mallants et al. (2017a) and include lateral transport under conditions of sloping soil layers. For pathways that deviate from the strictly vertical direction but still recharge into groundwater the resulting transport distances between source and groundwatertable would be longer, thus resulting in an additional reduction in concentration and hence would overestimate the exposure to a lesser degree than the purely one-dimensional approach. Furthermore, the required degree of information on the unsaturated zone hydrostratigraphy and the associated hydraulic properties for each stratigraphic layer, to allow use of two or three-dimensional models, would be prohibitive for a Tier 1 assessment. Nonetheless the current approach using one-dimensional geometry is the most conservative for a chemical assessment.

An exception could be made if the lateral transport through the unsaturated zone results in formation of so-called perched groundwater when water percolation is interrupted by another confining layer (clays or rock) thus forming a saturated zone (aquifer) above an unsaturated zone. However, perched aquifers are generally spatially limited and often shallow. Under those circumstances, chemicals will migrate laterally through such thin saturated layers and potentially be released directly into so-called flow-through wetlands, also known as upland swamps (Serov et al. 2012). A typical feature of such swamps is that water seeps through the upslope side and base of the wetland, and seeps back to the groundwater from the down slope side of the wetland. They occur in shallow basins or depressions located in low hills or mountainous regions. Because there is currently no indication of the existence of such swamps in the targeted study areas, this type of lateral solute transport will not be assessed.



Source: NSW Office of Water (2008)

Figure 5.4 Average groundwater level depths (based on 2008 data) for the Narrabri formation

Depth of the unsaturated zone describes the distance from the land surface down to the average groundwatertable and is a key parameter used to define the domain geometry (vertical length or depth). The depth is highly variable in the landscape as is evident from the groundwatertable map (see Figure 5.4). The average depth to shallow groundwater was also determined from groundwater level measurements available in the NGIS[9] database; depths vary from 1.7 m to 24 m (Area 1) and from 1 m to 27 m (Area 2). The average depth to the shallow watertable for the entire model domain is 21.3 and 17 m for Area 1 and 2, respectively. The depths to watertable vary over time. Some boreholes indicate declining water levels in the last 20 years (see the right hand side of bottom panel in Figure 5.5).

The decrease in groundwater levels for the Upper Namoi Alluvium as a result of groundwater extraction from coal seam gas aquifers and coal mining has been assessed to be less than 0.2 m in significant areas and between 0.2 and 2 m for other significant areas. The time of the maximum predicted drawdown is between 2010 and 2100 (SWS 2012c).

Groundwater discharge to the modelled rivers in the form of baseflow reduces steadily from 2010 until 2100. Compared to the base case model, it is predicted to be about 3 500 m^3/day less by the year 2100 (SWS 2012c).

The decrease in groundwater levels and river baseflow have not been accounted for in the current exposure assessment. The assessment assumes a long-term average groundwater level without any increase or decrease due to external factors (such as climate change, coal seam gas extraction, mining, agricultural extraction, etc). For stream flow, natural variation due to climate variability is accounted for. Any other long-term trend, whether increasing or decreasing, has not been considered.

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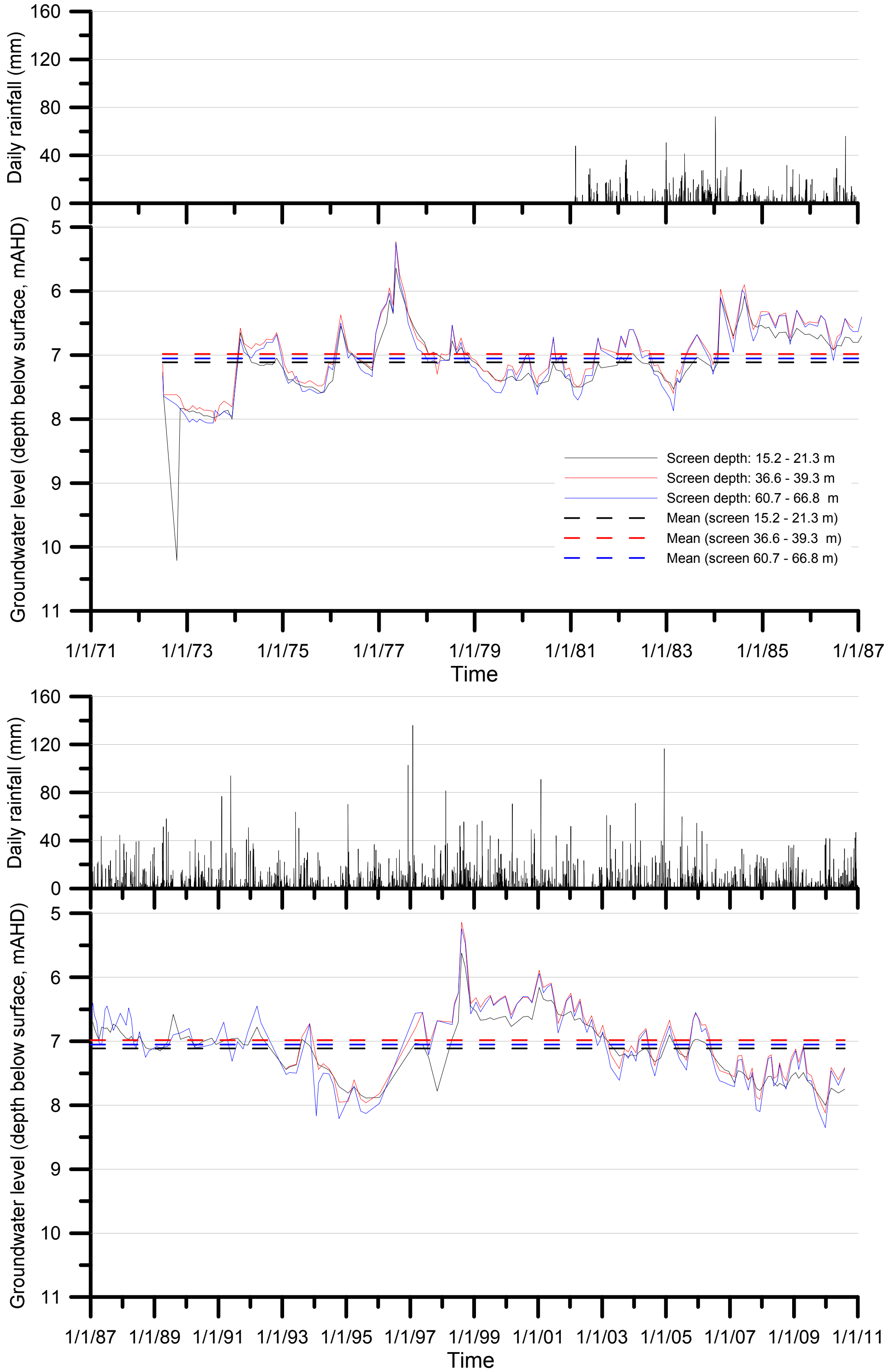
[9] http://www.ngis.com.au/ngisweb/

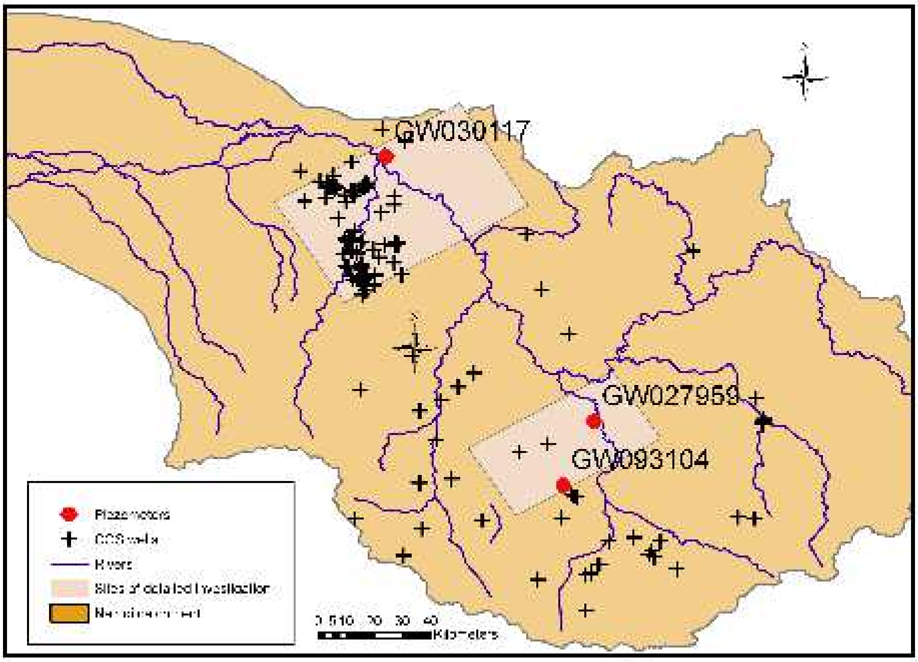
The exposure assessment will be simplified by performing solute transport calculations for the depth range 0 to 50 m, independent of the location of the source. In this way a concentration-depth (or dilution factor-depth) relationship can be established for further use. For existing coal seam gas sites, the relevant depth of the unsaturated zone can be derived from maps such as Figure 5.4, followed by derivation of the unsaturated zone dilution factor (DF_L) associated with that depth. The DF_L can be linked to the groundwater dilution factor (DF_{GW}) to calculate solute concentration in a receiving well. It is also possible to produce a simplified map displaying the spatial variation in groundwater dilution factor. This map allows a quick assessment of the dilution opportunities in different parts of the landscape, recognising several simplifying assumptions were invoked in its derivation to produce high end estimates.

A further simplification of the domain geometry relates to the assumptions made about how soil layers will be represented in the model. A complete soils map for the catchment at 1:100 000 scale was produced by the Namoi CMA, which had commissioned Soil Futures to produce this in 2008 (SoilFutures 2009). The soils mapping splits the catchment into 300 different areas. This level of detail is not required in the current phase of the exposure assessment, as the flow and solute transport simulations will directly use groundwater recharge as the key soil hydrologic parameter rather than using specific soil physical properties to calculate recharge. Higher tier assessments can use site specific soil information such as soil horizons and their respective soil hydraulic properties for recharge estimation. The available recharge data for the Namoi catchment are discussed in Section 5.2.4.



Source: Precipitation data: Jones et al. (2009); Groundwater data: BoM (2013). For location of wells see Figure 5.6.

Figure 5.5 Daily precipitation and groundwater levels, including long-term mean values, in selected multi-level shallow monitoring well GW030117



Source: BoM (2013)

Figure 5.6 Location of the monitoring well GW030117

5.2.3 Boundary conditions (including sources)

Consistent with Tier 1 assessment requirements, boundary conditions for water flow through the unsaturated zone were simplified by assuming a constant (time-invariant) groundwater recharge value. Groundwater recharge is a highly spatially variable parameter, and occurs via the Namoi River and its tributaries, especially during major flooding events, rainfall infiltration, irrigation, through flow from surrounding aquifers and catchments, and on-farm water losses. Finally, recharge can occur via upward leakage of groundwater from underlying aquifers (Welsh et al. 2014).

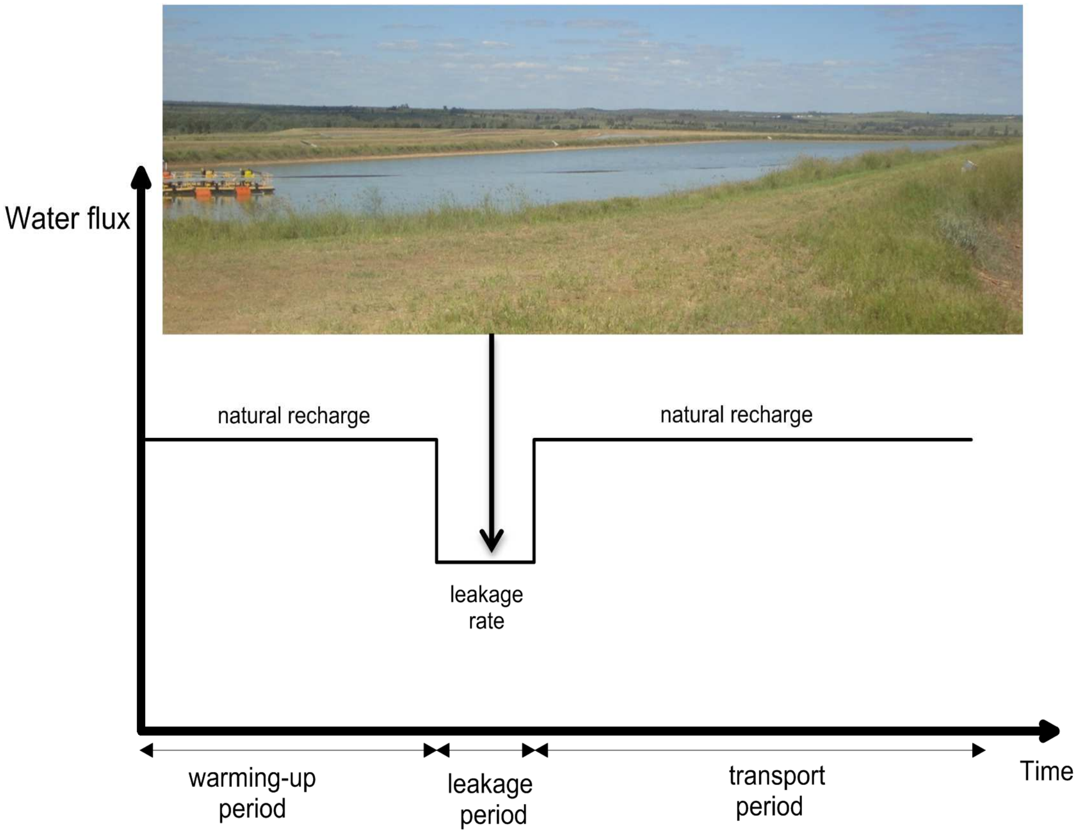
McNeilage (2006) reported average groundwater recharge in the Upper Namoi Groundwater Model to be 20 mm/y, although localised recharge from irrigation can be up to 72 mm/y. On the Liverpool Plains (coinciding with Area 2) average recharge varies from 5 mm/y with extremes between zero and 75 mm/y (Sun and Cornish, 2006) to 20 mm/y (Zhang et al. 1997), although the latter source also mentions up to 70 mm/y for the Sedimentary Hills. Lake Goran has an estimated recharge of 6 mm/y (Zhang et al. 1997). To simplify the exposure assessment, we will assume that the 20 mm/y recharge for the Upper Namoi Groundwater Model is the best estimate literature value available. The two areas considered for exposure assessment are part of the Upper Namoi Groundwater Model.

To account for uncertainty in the recharge values (see the above discussion), model simulations will consider three values: the best estimate (BE) from the literature (20 mm/y), a minimum value of 5 mm/y (BE/4), and a maximum of 80 mm/y (BE×4). The minimum and maximum are considered representative to capture the range of reported estimated values.

Leakage from a storage pond will assume two leakage rates: a reference value of 0.0032 m/y and a value ten times higher of 0.032 m/y (corresponding to 10^{-10} and 10^{-9} m/s, respectively, see Table 3.3). These leakage rates represent diffuse leakage over the entire surface area of the pond. The conceptual model assumes that there is a period with a constant natural recharge prior to the leakage period, and the leakage period is followed by a period with the same natural recharge (Source: CSIRO (Mallants et al. 2017a)

Figure 2.7

Figure 5.7). The first period allows the soil profile to achieve a steady-state water content along the entire unsaturated zone profile; this period is referred to as a 'warming-up' period. The last period is continued until the peak concentration is reached at the bottom of the unsaturated zone profile.



Note. Each period has a characteristic water flux. The leakage period corresponds to the depressurisation phase of Source: CSIRO (Mallants et al. 2017a)

Figure 2.7

Figure 5.7 Three periods are distinguished within the conceptual leakage model: a warming-up period, the leakage period, and the transport period

Boundary conditions for solute transport will accommodate all previously defined sources (point, line, areal source; see Table 3.3). A hypothetical unit concentration value will be used for the purpose of deriving dilution factors, travel times, fluxes and concentrations. Since all transport processes are linear, a simple rescaling allows the results obtained from a unit concentration to be rescaled for any other concentration.

5.2.4 Processes and parameters

5.2.4.1 Saturated and unsaturated water flow

Fluid flow through the unsaturated zone includes a number of components, such as inputs from precipitation and surface flows, and outputs from plant uptake via roots and transpiration, and evaporation from the soil surface (Table 5.2). Such processes are important in calculating water and solute movement to groundwater and their quantification is subject of considerable research (NRC 2000; Feddes et al. 2004). An important result from soil water balance calculations is the amount of water that infiltrates the soil and reaches the groundwatertable, which is termed recharge. The current approach simplifies this water balance calculation by imposing previously determined groundwater recharge rates on the solute transport model (see Section 5.1). Recharge will thus not be calculated but taken as a given (with reasonable uncertainty bounds, considering an uncertainty factor of 4 such that the minimum is 4 times smaller than the best estimate while the maximum is 4 times larger than the best estimate, see previous section). How this uncertainty is propagated through the process of calculating PECs is discussed in Mallants et al. (2017b).

Table 5.2 Summary of physical processes defining unsaturated water flow in soil and their relevance to Tier 1 and Tier 2

Process	Parameters	Included in Tier 1	Included in Tier 2
Precipitation	Daily rainfall/irrigation; land cover; slope of the land	Yes (simplified, implicitly accounted for via long-term mean recharge)	Yes (daily rainfall and / or irrigation rates)
Interception loss of precipitation from leaves	Throughfall rates	Yes (simplified, implicitly accounted for via long-term mean recharge)	Yes (simplified)
Surface flows and runoff	Flood volumes; runoff rates; rates of inflow/outflow to constructed water bodies	No	Yes (explicitly modelled)
Transpiration/root water uptake	Root distribution with depth	Yes (simplified, implicitly accounted for via long-term mean recharge)	Yes (explicitly modelled)
Transpiration/root water uptake	Root water uptake function	Yes (simplified, implicitly accounted for via long-term mean recharge)	Yes (explicitly modelled)
Evaporation	Evaporation rates; depth to the watertable	Yes (simplified, implicitly accounted for via long-term mean recharge)	Yes (explicitly modelled)

Note: Tier 1 = high end; Tier 2 = more realistic. For all chemicals that cannot be screened out via the Tier 1 assessment (i.e. cannot be removed from the list of chemical of potential concern), the Tier 2 processes would be invoked to produce more realistic and more site-specific recharge values. For unsaturated flow Tier 3 could be taken equal to Tier 2.

In reality, different soil materials (fine textured, coarse textured and mixtures of those) will result in different hydraulic conductivity (i.e. ability to transmit water) and water content profiles in the unsaturated zone (see e.g. Mallants et al. 2011). For the same water flux at the soil surface, such differences in water content will also result in different solute transport velocities. To account for these differences, two contrasting soil materials are assumed to provide a realistic though simplified representation of the natural variation in water contents, hydraulic conductivity and hence solute velocities for the same recharge rates. A sandy soil will represent the coarse textured materials, whereas a loam soil will represent the fine textured material.

The sand and loam soil are the two extremes in the exposure assessment, and represent a fairly broad range of hydraulic behaviour in unsaturated soil (see Figure 5.8). In terms of soil textural class, the loam soil is more representative than the sand for the soils within the Namoi alluvium. Dominant soil groups are grey, brown and red clays and black earths (Table 5.3). Despite their high clay content (45 to 70%), the grey, brown and red clays have a relatively high infiltration capacity as a result of cracking clay throughout the soil profile (Daniells et al. 1994). As discussed below, the USDA loam texture class used here in reality represents several textural classes in the Australian classification system. The results obtained with the loam soil are therefore considered as a reference, recognising however, that the unsaturated sediments underlying the soil may have different texture and structure and thus different hydraulic properties. Soil distributions in other bioregions will likely be different from the Namoi alluvium; nevertheless, the use of the sand and loam soil types do provide a broad range of hydraulic behaviour that would also provide high end estimates for other shallow groundwater areas.

Table 5.3 Major soil types in the Namoi alluvium

Soil type	**Constituent of Namoi alluvium (%)**
Grey, brown and red clays: heavy textured uniform clays	63.3
Black earths (chernozems): clay texture, with a good granular structure in the surface soil	23.9
Solodic and solodised soils: sandy to loamy surface	5.6
Red brown earths: loam to sandy-loam, surface soil overlying a reddish-brown clay subsoil.	3.6
Non-calcic brown soils	1.2
Euchrozems: friable dark brownish red clay loam at the surface	0.7
Lithosoils	0.5
Earthy sands	0.4
Other types	0.8

Source: NSW Office of the Environment and Heritage (2013)

By way of explanation, soil texture represents the relative composition of particles (sand, silt, and clay) in soil. The particle-size distribution is usually represented in a texture diagram, relating the percentages of sand, silt, and clay to a texture class. There are two major textural classifications used in the world; the International (ISSS 1929) and the USDA / FAO (FAO-UNESCO 1974) systems.

Particle-size limits used for clay are:

- < 2 µm for both the International and the USDA / FAO systems

For silt:

- 2 to 20 µm is used by the International
- 2 to 50 µm by the USDA / FAO system

And for sand:

- 20 to 2 000 µm is used by the International
- 50 to 2 000 µm by the USDA / FAO system.

Australia has adopted the International system. Both systems have adopted the same type of textural classes (12 in total; Australia has only 11 as the silt class is not considered), but the textural boundaries of these classes differ owing to the difference in boundary between clay-silt and silt-sand particles. As a result, classes from one system can have slightly different meaning in the other system. For example, a sand textural class of the USDA / FAO corresponds to at least three classes within the International (and thus Australian) system, i.e., Sand, Loamy Sand and Sandy Loam. The Loam textural class of the USDA / FAO corresponds to eight classes within the International system, i.e. Loamy Sand, Sandy Loam, Loam, Silt Loam, Clay Loam, Silty Clay Loam, Silty Clay, and Clay (Minasny and McBratney 2001).

Soil can be viewed as a complex system containing pores of various diameters. Water in those pores will rise to different heights due to capillary effects when a soil sample is placed in a water reservoir. The water in the pores will be held with different potential energies. Because each soil has a different distribution of pore sizes, the distribution of water above the water reservoir will also be different. This simple conceptual model assumes that soil pores can be represented by an equivalent bundle of capillaries with identical water retention properties as the real soil. Such an approach with capillary tubes and a water reservoir can be used to evaluate the water content distribution in a soil above the groundwatertable at equilibrium. The experimental curve that describes this relationship between the water content versus the height above the watertable is called the water retention curve. Many other names may be found in the literature, including pore water characteristic curve, capillary pressure-saturation relationship, and pF curve (Hillel 1998). The retention curve historically was often given in terms of pF, which is defined as the negative logarithm of the absolute value of the pressure head in centimetres. The water retention curve provides information on how tightly water is held in pores and how much work would need to be exerted to extract it from the different pores. The water retention curve thus characterises the energy status of water in the soil, and is one of the two soil hydraulic functions necessary to describe the status and movement of water in the vadose zone.

The most commonly used mathematical expression for the retention curve, $\theta(h)$, is the van Genuchten (van Genuchten 1980) equation since it permits a relatively good description of $\theta(h)$ for many soils using only a limited number of parameters. The van Genuchten soil moisture retention characteristic is defined as:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left(1 + |ah|^n\right)^m}$$

[Equation 6]

Where:

θ_r = the residual water content [cm^3cm^{-3}]

θ_s = the saturated water content [cm^3cm^{-3}]

α = shape parameter [cm^{-1}]

n = shape parameter [-]

m = $1–1/n$, shape parameters [-].

The dependency of the van Genuchten model on the soil hydraulic parameters is illustrated in Figure 5.8 for soil textural classes sand, loam, and clay.

The soil hydraulic properties for the analytical functions of van Genuchten (1980) associated with the sand and loam soils are taken from Carsel and Parrish (1988); they represent two out of the 12 textural classes of the USDA soil textural triangle (Table 5.4).

The second important soil hydraulic property is the *unsaturated hydraulic conductivity function*. The hydraulic conductivity characterises the ability of a soil to transmit water, and as such is inversely related to the resistance to water flow. The hydraulic conductivity depends on many factors, including the pore-size distribution of the porous medium, and the tortuosity, shape, roughness, and degree of interconnectedness of pores. The hydraulic conductivity decreases considerably as soil becomes unsaturated and less pore space is filled with water. The unsaturated hydraulic conductivity function gives the dependency of the hydraulic conductivity on the water content, $K(\theta)$, or pressure head, $K(h)$. The conceptual model that views the soil as a bundle of capillaries of different radii, as used earlier to explain water retention properties, may be used also to evaluate the hydraulic conductivity function. By adding the conductivity of all capillaries that are filled with water at a particular water content or pressure head, one obtains the hydraulic conductivity of the complete set of capillaries, and consequently of the soil itself.

Table 5.4 Soil hydraulic parameters for the analytical functions of van Genuchten (1980) for two textural classes of the USDA soil textural triangle

Properties		**Texture class**	
		Sand	**Loam**
Particle size		Must contain 85% or more of sand and % silt + 1.5x % clay must be less than 15%	Less than 52% sand; 28 to 50% silt; 7 to 27% clay
Soil hydraulic properties	Residual water content, θ_r [cm^3/cm^3]	0.045	0.078
	Saturated water content, θ_s [cm^3/cm^3]	0.430	0.430
	Shape parameter, α [cm^{-1}]	0.145	0.036
	Shape parameter, n [-]	2.68	1.56
	Saturated hydraulic conductivity, Ks [cm/d]	712.8	24.96

Source: Carsel and Parrish (1988)

Similarly, as for the water retention curve, analytical models are often used also for the hydraulic conductivity function. The van Genuchten (1980) retention function is similarly coupled mostly with the model of Mualem (1976) to give:

$$K(h) = K_s S_e^l [1 - (1 - S_e^{1/m})^m]^2 \qquad \text{[Equation 7]}$$

where:

m = $1–1/n$ ($n > 1$)

S_e = $(\theta - \theta_r) / (\theta_s - \theta_r)$

= effective saturation.

The pore-connectivity parameter was estimated by Mualem (1976) to be about 0.5 as an average for many soils.

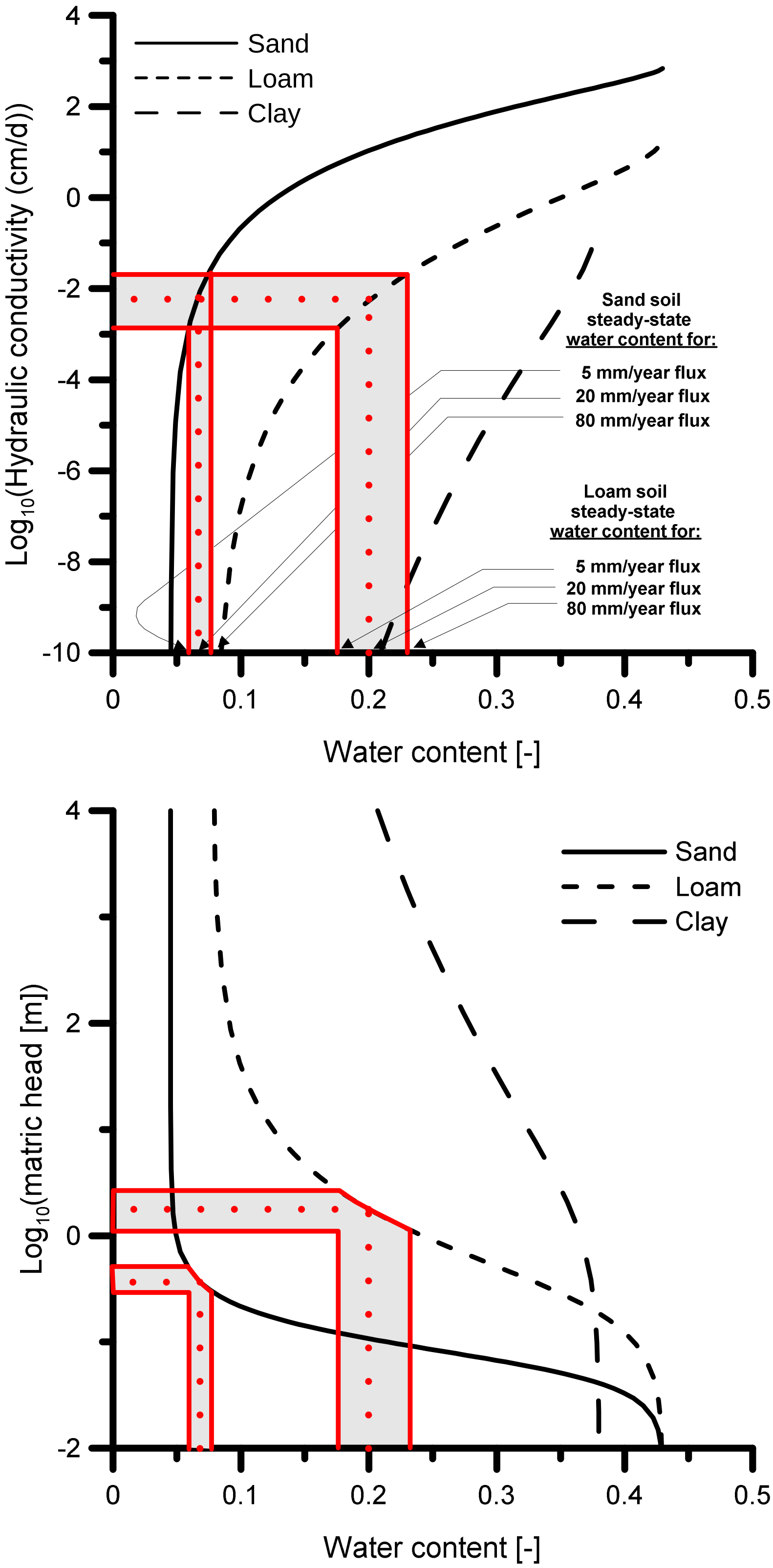
Figure 5.8 shows the combined water retention curve and the unsaturated hydraulic conductivity function for three soil textural classes (i.e. soil, loam and clay). Also shown are the steady state water contents corresponding to the imposed water flux at the soil surface (5, 20, or 80 mm/y).

The steady state water content within the soil profile, corresponding to a given water flux, can be obtained empirically via the unsaturated hydraulic conductivity graph such as the one in Figure 5.8. This is achieved by inserting the water flux on the hydraulic conductivity axis (e.g. the red dotted line on the Y-axis on the top graph of Figure 5.8 represents the 20 mm/y recharge), which is then connected to the unsaturated hydraulic conductivity curve, followed by dropping a vertical line onto the X-axis. The value on the X-axis defines the water content. The steady-state water content corresponding with 20 mm/y recharge is 0.2 cm^3/cm^3 for the loam soil.

The grey-shaded area represents the variation in soil water content, and thus a measure of the variation in solute velocity, which will be considered in the exposure assessments. The imposed variation in water fluxes at the soil surface (i.e. from 5 to 80 mm/y) results in a larger range of soil water contents for the loam (i.e. from 0.175 to 0.23 cm^3/cm^3) than for the sand (i.e. from 0.059 to 0.074 cm^3/cm^3) textural class.

For the relevant water fluxes considered in this exposure assessment (from 5 to 80 mm/y), the clay textural class would result in the largest steady-state water content of about 0.35 cm^3/cm^3 (not shown on Figure 5.8). Because solute pore-water velocity is inversely related to water content, the clay soil would yield the slowest velocity. As is shown by Mallants et al. (2017b), the slower the solute velocity, the higher the dilution or the lower the concentration at the bottom of the soil profile. In other words, an assessment that considers sand, loam and clay would likely overestimate the consequences the most for the sand and the least for the clay soil. An intermediate level of overestimation would be obtained for the loam soil. In the current exposure assessment, only the soil textures providing the two highest levels of overestimation are considered, i.e. sand and loam. This way high end estimates of solute behaviour can be derived.

As an example, Figure 5.9 displays the calculated equilibrium soil moisture content for sand- and loam- soil for three recharge rates: 5, 20, and 80 mm/y. For the reference recharge of 20 mm/y, the sand-soil has a water content of 0.065 $cm^3\ cm^{-3}$, while for the loam-soil the water content is 0.2 $cm^3\ cm^{-3}$. Because solute velocity is inversely proportional to soil water content (see Section 5.2.4.2), the same recharge rate in sand will have a 3 times larger solute velocity compared to loam. Figure 5.10 also shows that a sand soil is less sensitive to variations in recharge rate than a loam. Finally, leaching of chemicals is faster in sand than in loam, therefore, a sand soil will likely result in a higher exposure than a loam. This is not only true when the soil is not the receptor but only the pathway, but also when the soil is the receptor. This is demonstrated in Mallants et al. (2017b), as for any soil depth the sandy soil systematically gives higher concentrations (or lower dilution factors) than the loam soil.



Based on data from Carsel and Parrish (1988)

Figure 5.8 Example of hydraulic conductivity curves (top) and moisture retention curves (bottom) for the sand, loam and clay soil textural classes

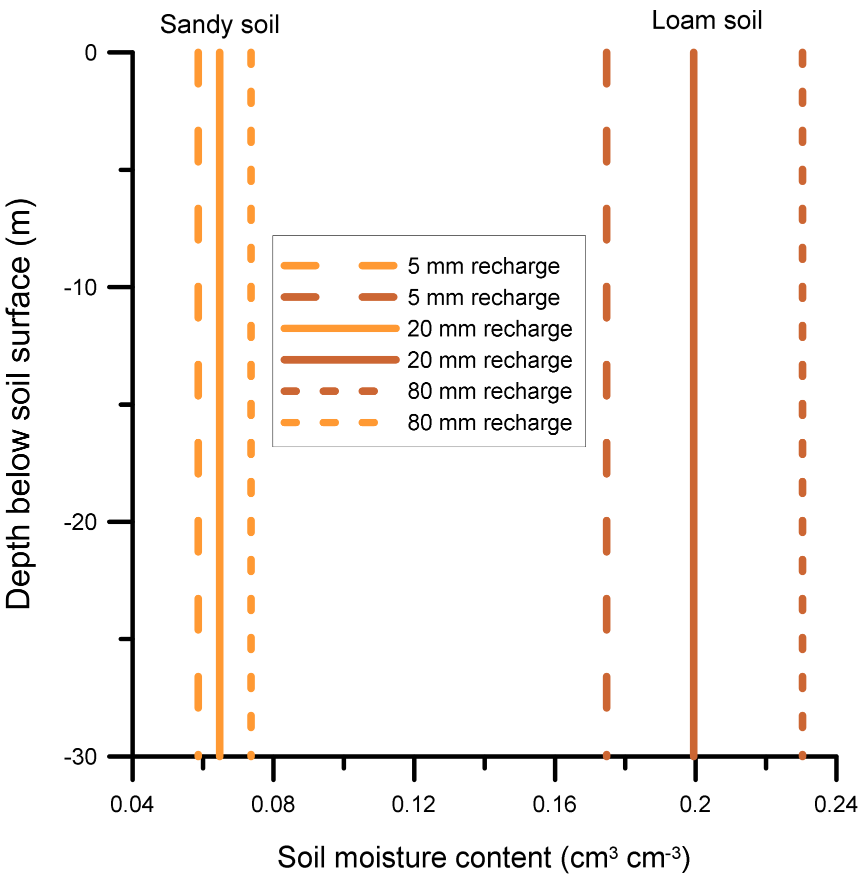


Figure 5.9 Calculated steady-state soil moisture content for sandy and loam soil subject to three recharge rates. For details of the calculations see Mallants et al. (2017b)

5.2.4.2 Chemical transport

Migration of chemicals in soil is primarily by advection and dispersion (ignoring gaseous transport). By mathematically solving the solute transport or advection-dispersion equation (ADE when advection is used or CDE when convection is used), predictions of solute concentrations at different depths and times will be obtained (Mallants et al. 2011). Transport calculations commensurate with a Tier 1 assessment are without chemical interactions between contaminants and the solid phases (clay minerals, organic matter, metal oxides) and without biogeochemical transformation (US EPA 2004b). A detailed discussion of processes relevant for Tier 1 and higher tiers can be found in Mallants et al. (2017a). The only physical processes accounted for in a Tier 1 assessment are advection (transport as a result of flowing water) and hydrodynamic dispersion (mechanical dispersion and molecular diffusion). Together with dilution or the mixing of dissolved chemicals with less concentrated water, these will thus be the only processes that will result in reducing the contaminant concentration while vertically migrating in the unsaturated zone (Figure 5.10). While solute advection is determined by the pore-water velocity v (v = soil water flux/soil water content or recharge/soil water content), dispersive transport is the combined effect of molecular diffusion and mechanical dispersion.

Diffusion or molecular diffusion is transport of solutes from an area of higher concentration to an area of lower concentration; it occurs as long as a concentration gradient exists between two locations in soil or groundwater, even if the water is not flowing. Mechanical dispersion is a transport process due to heterogeneous distribution of water flow velocities within and between different soil pores (Mallants et al. 2011). The result is that some solute particles will be ahead of the solute front whereas others will lag behind, leading to solute mixing and generally a bell-shaped distribution of velocities and thus of arrival times, typical of a breakthrough curve (Figure 5.10). The process of molecular diffusion and mechanical dispersion are incorporated into one parameter, the hydrodynamic dispersion coefficient *D*. Phenomenologically, dispersion has two effects: it increases the passage time of a solute pulse and it decreases the maximum concentration (Figure 5.10). In the case of a toxic contaminant for example, it leads to a longer exposure time but also to a lower maximum concentration.

In the unsaturated zone, advective transport usually is an important component of the overall transport, hence a two-component dispersion coefficient (*D*) (m^2/d) has to be used. Molecular diffusion (D_p) (m^2/d) is one component of the hydrodynamic dispersion, but unless water flow is extremely slow, molecular diffusion is of secondary importance[10] in the migration of elements in soils and permeable aquifer sediments. The second component being the mechanical dispersion (α x *v*):

$$D = D_p + \alpha \times v \qquad \text{[Equation 8]}$$

Where:

D	=	hydrodynamic dispersion, or simply dispersion
α	=	dispersivity[11] (m)
V	=	pore water velocity (m/d).

Dispersivity is a transport parameter that is often obtained experimentally by fitting measured breakthrough curves with analytical solutions of the advection-dispersion equation. For transport of inert, non-adsorbing contaminants during steady-state water flow the advection-dispersion equation (ADE) or convection-dispersion equation (CDE) is as follows (Toride et al. 1995):

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z} \qquad \text{[Equation 9]}$$

Where:

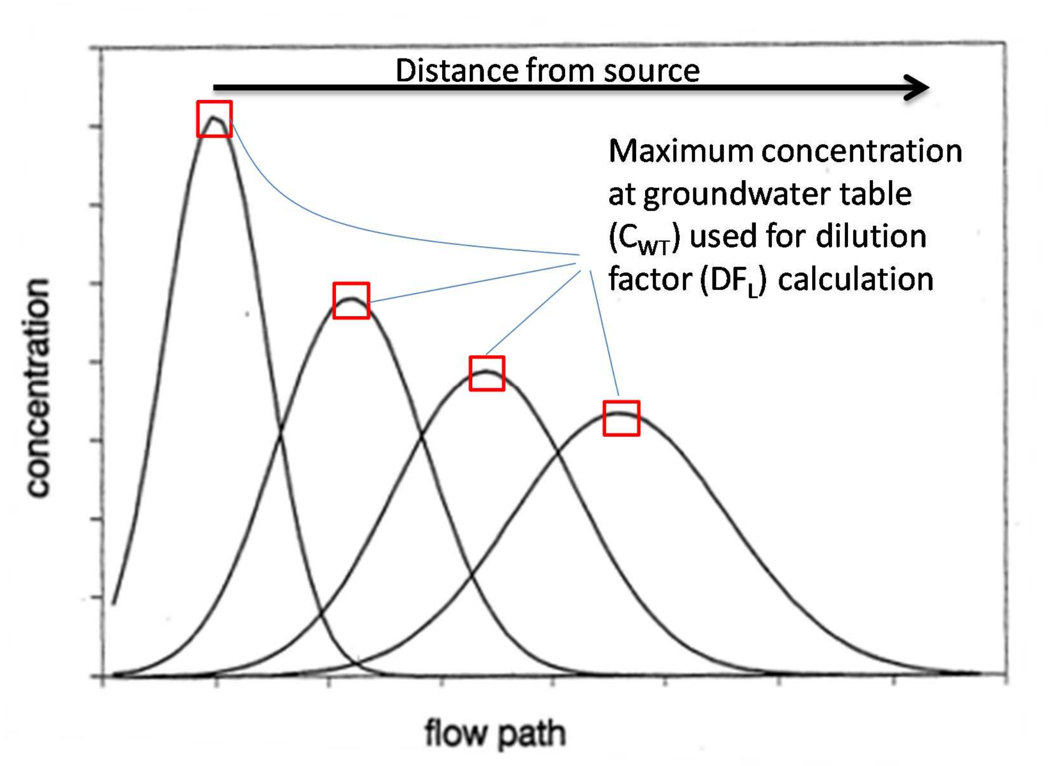
C	=	solute concentration in the water phase (mg/L)
T	=	time (d)
D	=	hydrodynamic dispersion (m^2/d)
Z	=	depth (m)
V	=	pore-water velocity (m/d).

For one-dimensional transport, and assuming solute transport is calculated in the main direction of flow, only the longitudinal dispersivity parameter (α_L) is relevant. For two-dimensional transport the transverse dispersivity parameter (α_T) is invoked and considers solute migration orthogonal to the main direction of flow. For three-dimensional

[10] Mechanical dispersion in most subsurface transport problems dominates molecular diffusion in the liquid phase, except when the fluid velocity becomes relatively small or is negligible. Diffusion dominated transport occurs in low permeability media, such as clays and rock matrices.

[11] Longitudinal dispersivity (α_L) is a term used to indicate dispersion along the main direction of flow.

transport the transverse dispersivity has two components: the horizontal transverse dispersivity (α_{TH}) and the vertical transverse dispersivity (α_{TV}).



Note. Maximum concentrations used to calculate soil dilution factor at interface with groundwatertable (=bottom of the soil profile). As distance from the source increases, concentrations decrease following increased mixing due to variations in flow velocities along the flow path.

Figure 5.10 Effect of advection and dispersion along a flow path (curves display different times) for a concentration along the solute flow path (from surface level through the unsaturated zone down to the groundwatertable)

The dispersivity often changes with the distance over which contaminants travel; this has been demonstrated through both theoretical analyses (Gelhar and Axness 1983) and field studies (Gelhar et al. 1985). For short transport distance, i.e. at the contaminant source, the value of α_L or D would be small, but it increases linearly until it reaches asymptotically its final value, the macroscopic dispersion D_A, after a transport distance X_L (Figure 5.11). Values of the longitudinal dispersivity usually range from about 0.01 m for relatively short, packed laboratory columns, to about 0.05 or 0.1 m for field soils (Vanderborght and Vereecken 2007). Longitudinal dispersivities can be significantly larger (up to hundreds of metres) for regional groundwater transport problems (Gelhar et al. 1985). If no other information is available, a good first approximation is to use a value of one-tenth of the transport distance for the longitudinal dispersivity, and a value of one-hundred of the transport distance for the transverse dispersivity when multi-dimensional applications are considered, given that the transverse dispersivity is typically one-tenth to one-hundredth of the longitudinal dispersivity (Anderson 1984).

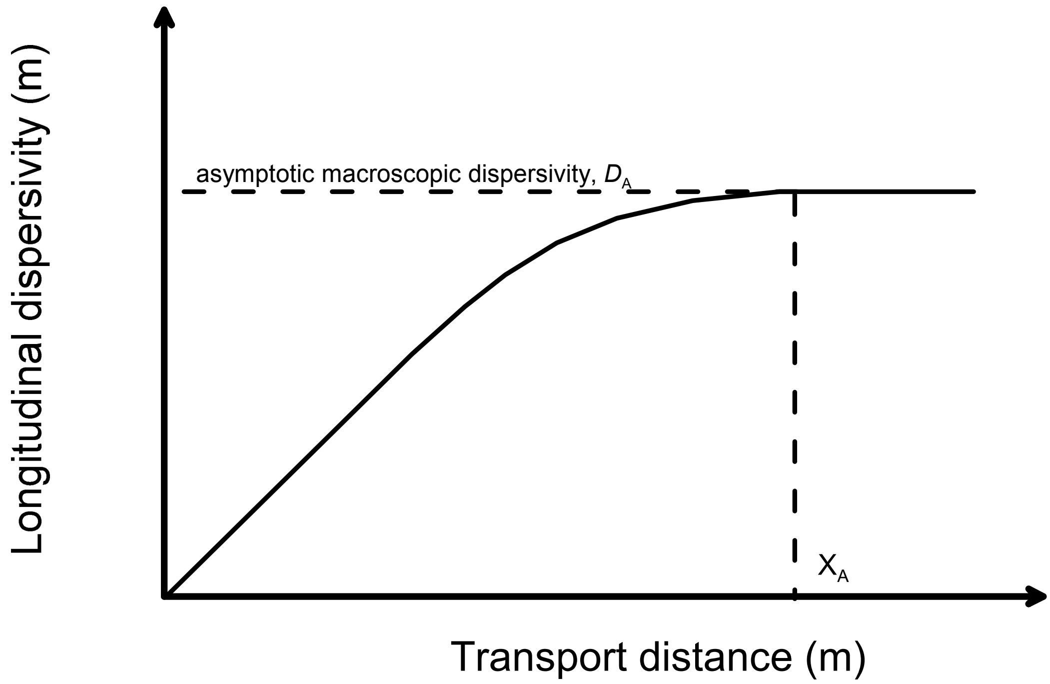


Figure 5.11 Longitudinal dispersivity versus transport distance

The approach adopted here for solute transport through unsaturated soil assumes the macroscopic dispersivity is reached after a transport distance of 5 m and the corresponding dispersivity is 0.1 m. This is based on the review of dispersivities for soils where for field tracer tests, the 75th percentile of dispersivity values was 0.1 m for both coarse and fine textured soil (Vanderborght and Vereecken 2007). The largest depth encountered in the reviewed field tracer tests was about 5 m; therefore, extrapolation of dispersivities for transport distances beyond this depth has to be done with care. A cautious approach is to consider a representative dispersivity value for the 5 m depth, here the 75th percentile value is chosen and subsequently applied throughout the remainder of the soil profile. While the dispersivity value of 0.1 m is smaller than a value of one-tenth of the transport distance for the longitudinal dispersivity (0.5 m in this case), this is acceptable as it overestimates predicted environmental concentrations (larger dispersivity values will decrease more the maximum concentration compared to small values), and such low values seem to better reflect the observed dispersivities for steady-state unsaturated flow in soil (Vanderborght and Vereecken 2007). For transport distances from 0 to 5 m a linear increase in dispersivity will be assumed, i.e. at x = 1 m α_L = 0.02 m, at x = 2 m α_L = 0.04 m, etc.

5.2.5 Receiving environments

Referring to Figure 5.2, two receiving environments are considered for the soil pathway: the soil-ecosystem, and the groundwatertable. The first receiving environment assumes that solutes are transported from a surface source into soil (unsaturated zone), with chemical concentrations being used to quantify consequences for soil ecosystems, mainly plants. The computational endpoints are solute concentration in soil water; and solute flux at the soil-groundwatertable interface. The second receiving environment considers solutes that reach the groundwatertable, become mixed with the shallow groundwater, and develop a plume which migrates with flowing groundwater and can be intercepted by deep-rooted plants. Computational endpoints for this situation include solute flux at the soil-groundwatertable interface, solute concentration in groundwater with minimum dilution (assuming a receiving well is within the source area), and unsaturated zone dilution factors (DF_L).

5.2.6 *Summary of calculation cases*

For both the 3-year and 30-year leakage from a surface pond, the calculations will consider eight soil depths and 18 parameter combinations, resulting in a total 2×144 calculation cases (as an example, Table 5.5 shows the 72 combinations for the 30-year leak for the loam soil). For each case, the dilution factor (DF_L) and the solute concentration at the bottom of the soil profile will be provided.

Table 5.5 Example of calculated dilution factors at the bottom of the loam soil profile for a 30-year leak from a surface pond (100 000 m^2) (from Mallants et al. 2017b).

	Loam soil								
Soil depth	Leak rate (mm/year)								
	0.35			3.5			35		
	Recharge rate (mm/year)			Recharge rate (mm/year)			Recharge rate (mm/year)		
	5	20	80	5	20	80	5	20	80
1 m	7.8	8.8	9.9	1.1	1.2	1.2	1.0	1.0	1.0
2 m	15.7	17.7	20.3	1.7	1.9	2.1	1.0	1.0	1.0
3 m	23.6	26.8	30.7	2.5	2.8	3.1	1.0	1.0	1.0
4 m	31.5	35.8	41.2	3.2	3.6	4.1	1.0	1.0	1.0
5 m	40.6	46.2	53.2	4.1	4.7	5.4	1.0	1.0	1.0
10 m	58.2	66.4	76.5	5.9	6.7	7.7	1.1	1.1	1.1
20 m	83.0	94.6	109	8.3	9.5	10.9	1.2	1.2	1.3
30 m	101	115	133	10.1	11.6	13.3	1.3	1.4	1.5

For point sources, detailed concentration profiles will be calculated for the first 0.5 m of the unsaturated zone. For a small point source, the results will be provided 1, 10 and 100 days after the spill occurs (for sand and loam soil). A spill of 3.8 L will be assumed to infiltrate a surface of 1 m^2 in 1 hour. The same concentration versus depth information will be provided for the large point sources; a spill of 15 000 L will be assumed to infiltrate a surface area of 10 m^2 during 16.4 days (taking the same infiltration rate as for the small source: 3.8 L/h).

Dilution factors and solute concentrations obtained through Table 5.5 will be used to construct empirical distribution functions for each soil depth. In this way the results can be summarised in a statistical way, from which any percentile value (such as the 95thpercentile) can be then derived for assessments.

5.3 Groundwater pathway

5.3.1 *Rationale for a regionalised generic approach*

The usefulness of a Tier 1 assessment with a generic groundwater model is limited when the results need to be representative of a broad set of hydrogeological conditions. In the context of the National Coal Seam Gas Chemicals Assessment, such a broad set of hydrogeological conditions refers to the priority bioregions agreed by the Australian Government. Rather than developing several region-specific groundwater models, a complex undertaking that is not necessary in a Tier 1 approach aimed at delivering high end estimates, a limited set of groundwater flow models in a single sub-bioregion will be developed. These models can then be used as a basis for more detailed groundwater transport calculations to derive precautionary, high end predictions of environmental concentrations. This regionalised generic approach uses a single conceptual model with a broad range of parameter values. This kind of approach also allows a high throughput evaluation of chemicals (i.e. efficient analysis of a large number of chemicals) while still considering a broad range of hydrogeological conditions.

The regionalised generic approach considers the following elements:

- out of the two proposed areas from within the Namoi catchment, one area was selected as the basis for developing smaller and a more detailed sub-domain model for solute transport calculations. The selection was based on:
  - potential risk based on ongoing and planned activities in regards to coal seam gas extraction
  - being sufficiently representative in terms of broad coverage of hydrogeological features
  - being sufficiently representative in terms of receiving environments of relevance to both human and environmental receptors.
- solute transport calculations were run with the sub-domain model within the selected subregion. The groundwater model with calibrated parameters (see Chapter 4) will serve as reference case and currently represents the best available information about the shallow groundwater in the alluvial aquifers within the Namoi catchment.
- additional simulations of the models were undertaken by perturbing the reference set of hydrogeological parameters (hydraulic conductivity, hydraulic gradient[12], effective porosity) according to the distribution of such parameters encountered in the subregions model. In this way, a set of outputs were generated that were representative for the entire subregion, as the sub-model, being only a few km^2 in size, could not capture the entire range of groundwater flow velocities that exist within the entire subregion. This perturbation approach is similar to a sensitivity analysis involving multiple parameter combinations.
- receiving environments such as shallow aquifer observation wells were considered at different distances from the source to quantify the degree of dilution as a function of distance.
- The output from this analysis, assuming a hypothetical solute source concentration, is a set of concentrations for each of the identified receiving environments from which parameters such as dilution factors can then be calculated.
- Concentrations over time and space can also be derived.
- If spatially enabled, this form of 3D modelling of predicted concentrations can also facilitate the generation of probabilities of occurrence, which in effect quantify the likelihood of the solute encountering specific receptors at specified distances and/time periods from the point of release.

The dilution factors can subsequently be used to derive solute concentrations for specific chemicals once their source concentration is known. The dilution factors can be arranged in

[12] Indirectly by changing the river bed conductance.

a lookup table facilitating further use to derive empirical distribution functions of dilution factors, and for a specific location in a real site without the need to redo the impact assessments for that site (Table 5.6). The example provides dilution factors as a function of distance to well, hydraulic conductivity for porous and fractured aquifers (low, medium and high values), and hydraulic gradient (low, medium and high). There can be any number of classes for each parameter, and there can be additional parameters such as effective porosity, depth of the unsaturated zone and the associated dilution factors (see Figure 5.12). The lookup tables will be developed in Microsoft Excel worksheets and will become a practical tool for regulators and other end-users.

The lookup tables present discrete outputs in terms of combined dilution factors for the unsaturated zone, groundwater wells, or other receiving environments. The various lookup tables are provided in Mallants et al. (2017b). On the basis of the dilution factor-to-soil depth or dilution factor-to-travel distance relationships, additional dilution factors can be generated in between the discrete outputs.

Lookup tables can be used in different ways, depending on the desired degree of overestimation of the analysis. The highest overestimation would result from taking the overall lowest dilution factor across all parameter values (hydraulic conductivity, hydraulic gradient, and porosity) for a given well distance (taking the well receiving environment as an example) from the lookup table. This approach would disregard use of site-specific information about the groundwater flow to help select the appropriate parameter combination and the associated dilution factor.

The second approach would make use of a cumulative probability distribution that can be generated from all dilution factors for a given well distance. If three parameter values (low, medium, high) are considered for each of the parameters (hydraulic conductivity, hydraulic gradient and porosity), the number of parameter combinations can be determined by equating 3 × 3 × 3. As this equals 27, there will be a 27 resultant dilution factors evaluated. From such a set of dilution factors probability distributions can be constructed from which any percentile can be chosen for further analysis.

Table 5.6 Example lookup table with dilution factors in groundwater (*DF*11, *DF*21, ...) for different values of hydraulic conductivity and hydraulic gradient (L=low, M=medium, H=high)

	Hydraulic conductivity K									
	Porous aquifer									Fractured aquifer
	Low *K* (clay)			Medium *K* (silt)			High *K* (sand/gravel)			Fracture permeability L, M, H
	Hydraulic gradient *i*			Hydraulic gradient *i*			Hydraulic gradient *i*			
	L	M	H	L	M	H	L	M	H	
Distance to well	***Dilution factor***									

	Hydraulic conductivity K									
100 m	DF11	DF12	DF13	DF14	DF15	DF16	DF17	DF18	DF19	
200 m	DF21	DF22	DF23	DF24	DF25	DF26	DF27	DF28	DF29	
…										
500 m	DF51	DF52	DF53	DF54	DF55	DF56	DF57	DF58	DF59	
1000 m	DF11	DF12	DF13	DF14	DF15	DF16	DF17	DF18	DF19	

The third approach would allow for a more differentiated analysis making use of available information about broad classes of sediment materials, hydraulic gradients etc. The assessor would use such information to limit the number of parameter classes from which to choose the dilution factor. As a result, not necessarily the most conservative dilution will be selected.

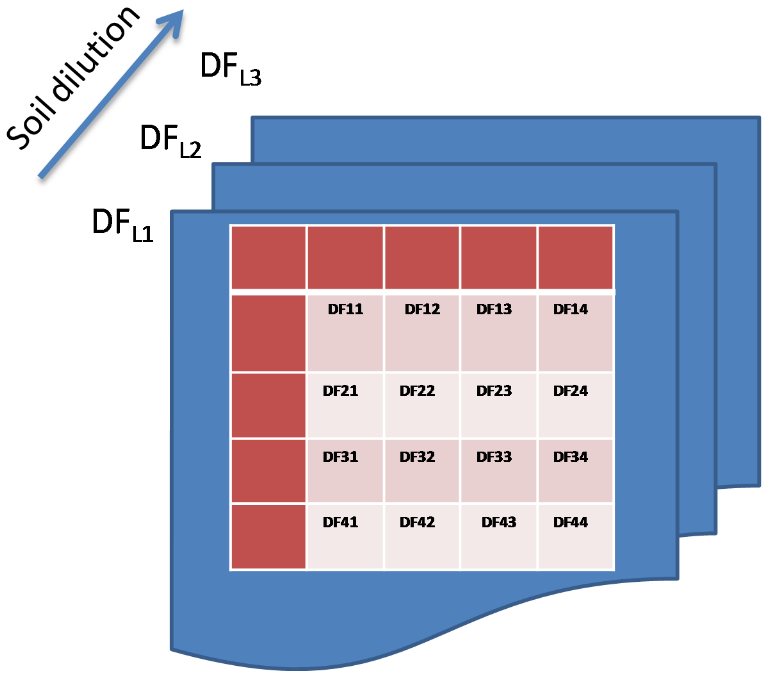


Figure 5.12 Lookup table displaying the combined soil dilution (DF_{Lxx}) and groundwater well dilution factors (DF_{xx}). Similar lookup tables can be derived for other receiving environments

5.3.2 Receiving environments

Exposure assessments carried out in the framework of the National Coal Seam Gas Chemicals Assessment consider both human exposure (public and occupational[13]) and exposure of the environment. Human health public exposure is mainly through contamination of ambient air, drinking water and recreational water (e.g. lakes). Drinking water may be derived from groundwater and / or surface water. In regards to occupational exposure of workers at the coal seam gas site or during transport of chemicals, dermal and inhalation exposure to chemicals may occur (NICNAS 2017a). For this purpose, chemical concentrations in soil following a spill at the coal seam gas site will be calculated (for details, see Mallants et al. 2017b).

[13] direct exposures at the workplace.

The receiving environments for the environmental exposure assessment include:

- soil water
- shallow groundwater, including groundwater accessible by groundwater dependent ecosystems
- rivers receiving discharge from shallow groundwater, or 'gaining rivers'
- wetlands that are either connected or disconnected from rivers and that are continually or intermittently dependent on groundwater (DoEE 2017b)
- and springs (note that due to the large distance between springs in the Namoi and coal seam gas wells, see Section 5.3.2.4, conceptual models for springs will not be developed)

Human exposure assessments for the public typically combine several exposure pathways as depicted in Figure 5.13, such as:

- uptake of food products including meat, milk, vegetables, and cereals
- drinking contaminated water
- inhalation of gaseous / volatile contaminants
- direct skin exposure from swimming or bathing in contaminated water

In the National Coal Seam Gas Chemicals Assessment, only oral exposure via drinking water, dermal exposure via recreational water, and inhalation exposure via air and dust are considered (NICNAS 2017b). In other words, any exposure pathway associated with ingestion, such as consumption of produce originating from livestock (e.g. milk, meat) or crops (e.g. vegetables, cereals) has been excluded from the conceptualisation. The main reason for this simplification is that currently no data are available on levels of chemical residues in food which could be linked to contamination by drilling and hydraulic fracturing operations. Therefore, because of the difficulty in establishing likely levels of contamination of foods linked to these operations, public exposure to drilling and hydraulic fracturing chemicals via food is not quantified in the current exposure assessment. In absence of real data on chemical residues in food produce, chemical concentrations of residues can be calculated using so-called biosphere or environmental transfer models (IAEA 2004; Pröhl et al. 2005; Perko et al. 2009a). Such calculations were beyond the scope of the current study.

5.3.2.1 Drinking water

In case of public exposure, uptake or ingestion of contaminants will be considered from drinking water produced from groundwater or surface water. In the considered Namoi catchment, the current fraction of drinking water produced from groundwater / surface water is about 50 / 50 (CSIRO 2007). In years of minimum surface water diversions, current levels of groundwater use represent 78% of total water use. By 2030 the groundwater use would represent 60% of total water use (CSIRO 2007). Assessment scenarios will assume drinking water is produced either 100% from groundwater or 100% from surface water. These two scenarios represent two extreme cases or 'end members' regarding chemical concentrations. Based on these two end members, the chemical concentrations for any groundwater-surface water ratio could be calculated.

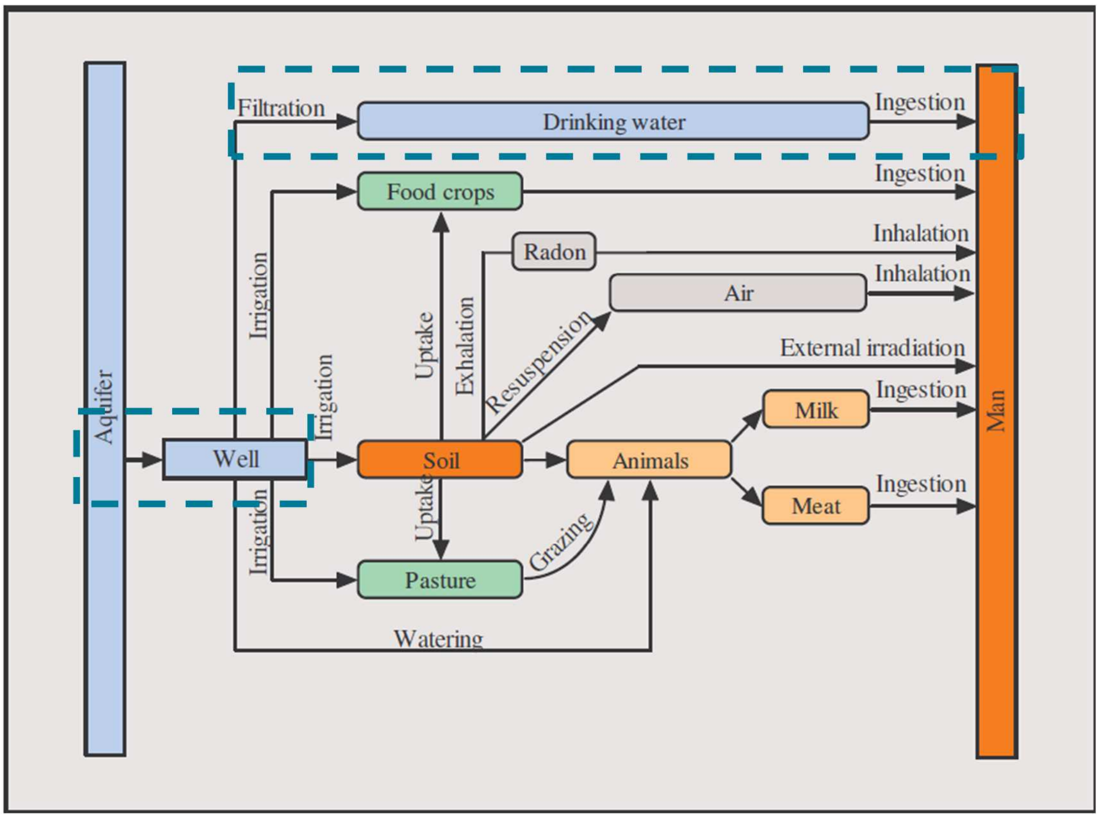
Drinking water produced from groundwater

Groundwater extraction is mainly from the shallower Narrabri and deeper Gunnedah formations (generally between 40 to 90 m), which make up the alluvial aquifers (they occupy 7 334 km^2 out of 42 064 km^2 for the entire catchment area). For our assessments only water supply bores screened over a depth less than 50 m will be considered. The number of such shallow bores (filter depth less than 50 m) for drinking water production (assumed equal to domestic and town supply) in the alluvial aquifer is 4 560 in the modelled study (Domestic and Town supply, Table 5.7), with a density of 0.62 bores/km^2.

Table 5.7 Number of water wells (screen depth less than 50 m) in the catchment (total area) and in the alluvial aquifers (Narrabri and Gunnedah formations)

Water use	Number of wells in total area	Number of wells in alluvial aquifer
Irrigation	6 305	4 837
Farming	414	210
Stock	15 638	6 984
Industrial	205	89
Mining	55	8
Domestic	10 135	4 392
Town supply	249	168
Other (Oil exploration, fire fighting, commercial etc.)	1 250	213
Total	***34 215***	***16 893***

Source: NSW Government (2014a)



Groundwater contaminants enter the drinking water well and will give rise to exposure via ingestion, inhalation and external exposure (e.g. external irradiation from soil contaminated with naturally occurring radioactive *materials (NORM) associated with drilling and water management; IAEA 2003b). Only the exposure pathway via drinking water is considered in the National Coal Seam Gas Chemicals Assessment.*

Figure 5.13 Typical exposure pathways considered for a groundwater bore scenario

Predicted environmental concentrations from water supply bores will be obtained by assuming hypothetical wells that penetrate several aquifer layers and whose concentrations in pumped well water is equal to the groundwater concentration calculated at the specific well location and well depth. This concentration will be a weighted average of the concentrations along the entire screen depth. The model will not assume a specific pumping rate; this is generally an assumption leading to high end estimates as pumping will result in additional dilution when uncontaminated water is mixed with contaminated water. The hypothetical wells will be located at increasing distances from the surface source such that distance-concentration relationships can be derived. An efficient way to deal with different source concentrations (for different contaminants) is to calculate a single dilution factor which is then used to rescale source concentrations to groundwater concentrations. This approach is followed here.

Drinking water produced from surface water

Surface water from streams is also used for the production of drinking water. The contaminant concentration in the stream will be calculated by assuming the following dilution of the contaminant flux into the river:

$$Concentration = \frac{Contaminant\ flux\ into\ river\ (mg/year)}{Groundwater\ discharge\ into\ river\ (L/year)} \qquad \text{[Equation 10]}$$

Since the contaminant flux into the river is through groundwater discharge, only river sections that are connected to groundwater and gaining are considered.

5.3.2.2 Recreational water

Recreational water is surface water in the form of rivers, tributaries and anabranches, dams or lakes. For such a receiving environment to be relevant it must be established whether a connection with groundwater exists. If such is the case, then the approach for estimating solute concentrations will depend on the type of surface water, i.e. stream or lake / dam. For a stream the approach described previously for estimating solute concentrations in surface waters after discharge of contaminated groundwater will be followed. In other words, Equation 7 will be applied using the relevant stream discharge. In the case of a dam or lake, the approach will consider groundwater discharge into the wetland or dam.

5.3.2.3 Water wells

The conceptualisation of contamination of drinking water produced from groundwater will use a weighted average of simulated concentrations along the filter section of the water well to determine the concentration at a given well. The model will not assume a specific pumping rate. The calculations will assume hypothetical wells placed at increasing distance from a source. This will provide information on how concentrations (and thus impact) decrease with increasing distance. The next step is to define the number of water wells within a given distance from a coal seam gas well; it is assumed for reasons of simplicity that the coal seam gas well is the location where the leak or spill occurs. This allows determination, for the currently known locations of coal seam gas and water wells, of the likelihood of a water well being within a potential contamination plume. This distance-likelihood function can be linked to the distance-consequence[14] relationship obtained from the transport simulations.

Table 5.8 Number of shallow wells (up to 50 m deep) located in the vicinity of the coal seam gas wells. Total number of the shallow wells is 34 215

Radial distance from the nearest coal seam gas well (m)	Number of shallow wells	Cumulative number of wells	Percent of the total number of shallow wells (%)	Cumulative probability (%)
100	10	10	0.03	0.03
200	24	34	0.07	0.10
500	116	150	0.34	0.44
1 000	300	450	0.89	1.33
2 000	928	1 378	2.7	4.03
5 000	4 310	5 688	12.6	16.63
10 000	12 003	17 691	35.0	51.63

Source: NSW Government (2014a)

This is similar to hypothesis testing in that a test can be performed on whether the possibility of a hypothesised impact occurring can be rejected with a high probability. For instance, a typical hypothesis could be one that considers contamination of a domestic bore 500 m from the coal seam gas well. Hypothesis testing enables the rejection of the possibility of such an occurrence with high probabilities such as 95 or 99%. The number of shallow wells (up to 50 m deep) within a short distance from the existing coal seam gas developments is shown in Table 5.8. The wells have different uses, such as for irrigation, stock, and domestic applications. No distinction was made between these three well types in the current analysis.

The corresponding empirical cumulative distribution function of wells within a given distance from the nearest coal seam gas well is shown in Figure 5.14. Note that only wells within a distance of 10 000 m have been considered. This represents 17 691 (52%) out of a total of 34 215 wells considered in Table 5.8. The cumulative distribution reveals there is only a 1% chance of finding water wells within a distance of approximately 600 m of a coal seam gas well, or conversely, in 99% of all cases wells will be at distances greater than approximately 600 m from a coal seam gas well. The closest distance reported between a coal seam gas and water well is 100 m. The probability of this occurring is only 0.03% (10 out of a total of 34 215 wells), which corresponds to 3 times out of 10 000 (see Table 5.8).

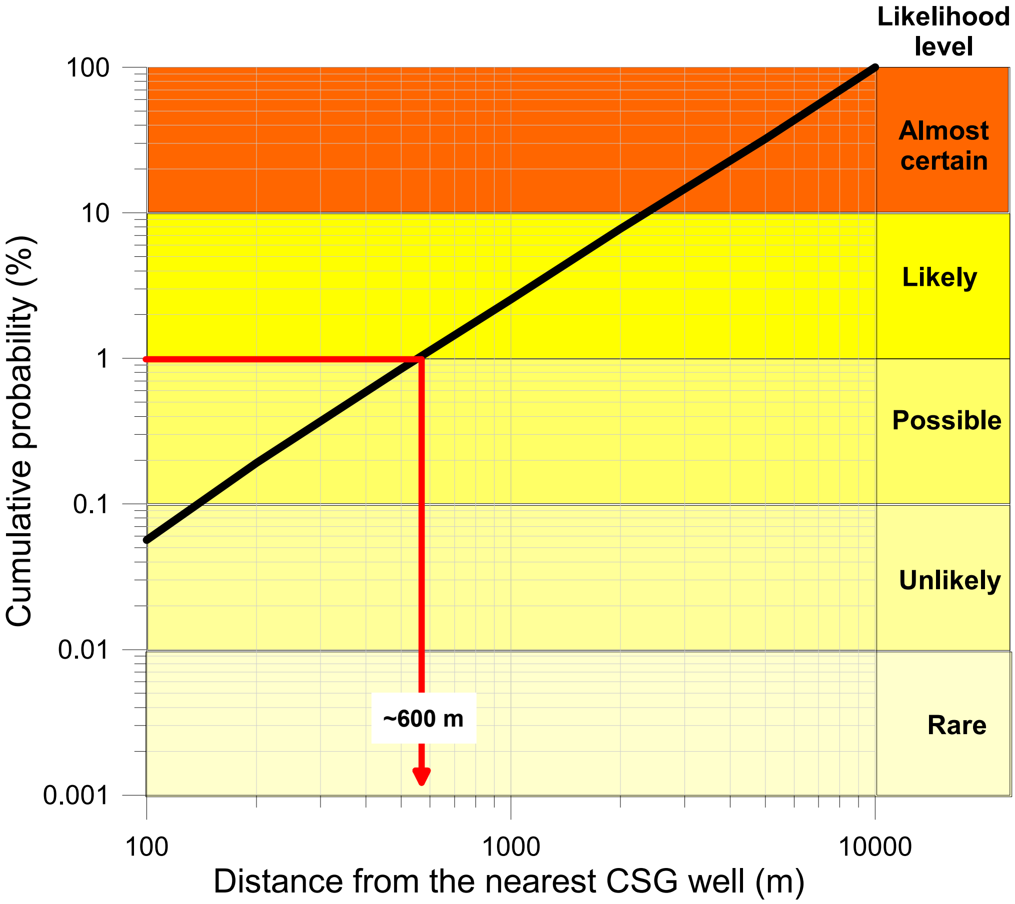
The cumulative probabilities can be converted into likelihood levels using the following probability levels (see also Figure 5.14):

- almost certain (100–0%)
- likely (10–1%)
- possible (1–0.1%)

[14] Based on distance-dilution factor relationship, a distance-consequence relationship can be developed for a given chemical with known or assumed source concentration

- unlikely (0.1–0.01 %)
- rare (0.01–0.001%)

Applying these levels to our particular data from Figure 5.14, we can state that it is unlikely to find water wells within 100 m of coal seam gas wells. Combination of the likelihood levels with consequence levels (e.g. arranged in five classes with consequence levels from 1 to 10 000) allows construction of a risk matrix (DRET 2008).



Note. Likelihood levels can be used to develop a risk matrix (see Figure 2.2).

Figure 5.14 Empirical cumulative distribution of water wells at a given distance from the nearest coal seam gas well

The locations of water wells in the two local models are shown in Figure 5.15 and Figure 5.16. These include bores that are pumped for town water supplies, domestic, farming, stock and irrigation purposes.

5.3.2.4 Discharge areas (springs, rivers, wetlands)

The receiving freshwater environments considered comprise an extensive range of aquatic habitats including swamps, floodplains, wetlands, streams and rivers. The Atlas of Groundwater Dependent Ecosystems (BOM 2013) presents the current knowledge of groundwater dependent ecosystems across Australia and is an important source of information to locate the receiving environments. Of relevance are ecosystems such as springs, wetlands, rivers and vegetation that interact with groundwater. Additional sources of information to identify location of receiving environments are the NSW *Threatened Species*

Conservation Act 2013 and the *Environment Protection and Biodiversity Conservation Act 1999* (EPBC Act).

Shallow groundwater

Exposure pathway is via direct uptake of groundwater by plants that can access groundwater. Such plants access water via the capillary fringe or vadose zone, i.e. the subsurface water just above the watertable that is not entirely saturated. Direct uptake from the watertable is not believed to be common because plant roots do not easily grow under saturated conditions as oxygen is required for plant respiration and growth. In theory, the greater the depth to groundwater the less the dependence will be of vegetation on groundwater. However, if groundwater can be accessed, ecosystems will likely develop some degree of dependence (Hatton and Evans 1998).

Data for Australian plant species suggests that at depths greater than 10 m the groundwater dependency decreases and / or is minimal (Eamus and Froend 2006). A simple rule of thumb is therefore to assume that in those areas where the watertable is less than 10 m below the surface, vegetation will be groundwater dependent. Conversely, vegetation is less likely to depend on groundwater in regions where the water table exceeds 10 m, although there is evidence that some Eucalyptus species possess roots up to 60 m deep (Le Maitre et al. 1999).

A more systematic and evidence-based assessment of groundwater interaction with ecosystems is available from the Atlas of Groundwater Dependent Ecosystems (GDE), which allows for determination of the currently known locations of coal seam gas and water wells and the likelihood of a water well being within a potential contamination plume. The GDE Atlas expresses the likelihood for ecosystems to access groundwater for the following two GDE layers: ecosystems that rely on the subsurface presence of groundwater (vegetation), or ecosystems that rely on the surface expression of groundwater (rivers, wetlands, springs). Three categories of GDE potential were mapped within each of the GDE layers (normalised values from 1 to 3 were used to indicate likelihood of groundwater interaction):

- high potential for groundwater interaction (rating 3)
- moderate potential for groundwater interaction (rating 2)
- low potential for groundwater interaction (rating 1).

These GDE potential categories indicate the potential for each ecosystem to be interacting with groundwater, based on the physical landscape and ecosystem characteristics. For example, a shallow watertable, constant evapotranspiration (ET) in dry periods, or known groundwater using vegetation are physical characteristics of an ecosystem that suggest the potential for groundwater interaction is high. Conversely, vegetation growing over deeper watertables, with seasonal ET would suggest that the potential for groundwater interaction is lower. A low potential for groundwater interaction means that ecosystems are relatively unlikely to be interacting with groundwater. This will include ecosystems that are not interacting at all with groundwater. High potential for groundwater interaction means that there is a strong possibility that ecosystems are interacting with groundwater.

The three GDE categories are displayed in Figure 5.21 for ecosystems that are dependent on surface and subsurface expression of groundwater. For the purpose of assessing the probability of such ecosystems to become contaminated by chemicals present in groundwater, each category of groundwater interaction is converted into a category of potential contamination. In other words, the GDE category with ranking 3 equates to an ecosystem with high probability for contamination, while ranking 1 would indicate low probability for contamination. A risk analysis matrix can then be developed by combining probabilities or likelihood with consequences (e.g. catastrophic, moderate, insignificant). The consequence would be based on an evaluation of the impact of chemical concentrations in the soil root zone on ecosystems. Concentration in the soil root zone may be assumed equal to the concentration in the shallowest groundwater (model) layer.

Rivers receiving discharge from shallow groundwater (gaining rivers)

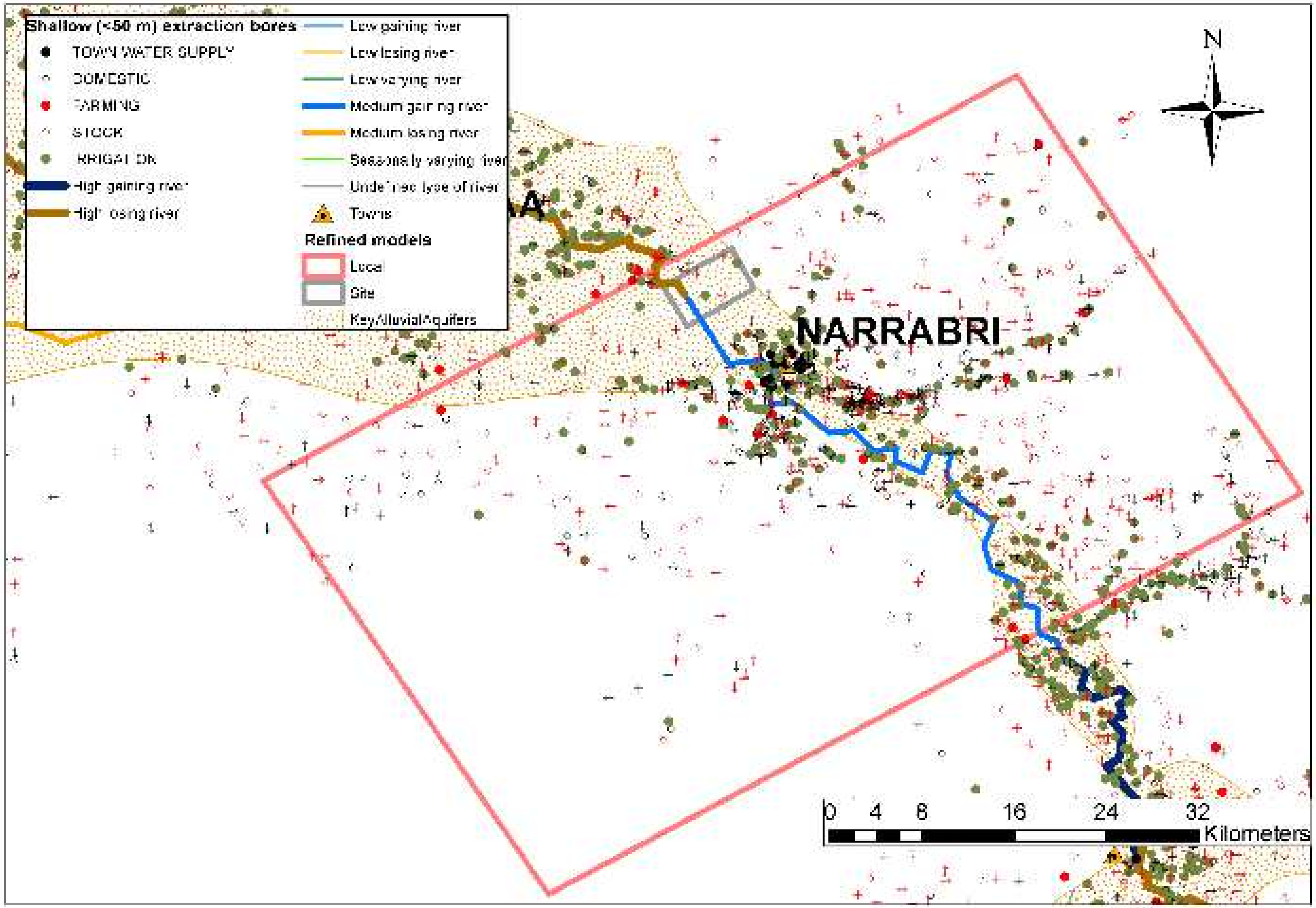
Exposure pathway is via contact with river water. Shallow groundwater and contaminants are discharged into gaining river sections. A considerable dilution in concentration is expected as groundwater contribution is usually a relatively small fraction of total stream flow, especially at higher flows. The likelihood of a contaminant plume discharging into a gaining river also depends on the groundwater flow direction in the vicinity of the river. If groundwater flow lines are orthogonal to or at an acute angle to the river any plume within those flow lines will likely discharge into the river. If flow lines are more parallel to the river, a situation that can occur if the river is not hydraulically connected to the groundwater, the likelihood for contamination of the river is small. By means of particle tracking using the MODPATH simulator, flow paths can be generated from existing coal seam gas wells to visualise the potential connection with rivers or other receiving environments.

Lakes

Surface water bodies such as lakes and ponds being fed by groundwater will potentially become contaminated and hence provide a potential contamination pathway in case of recreational water use. The currently identified modelling areas do not have lakes or similar water bodies where such exposure might occur. The exposure assessment will therefore be based on a theoretical lake with theoretical volume and hence dilution capacity.

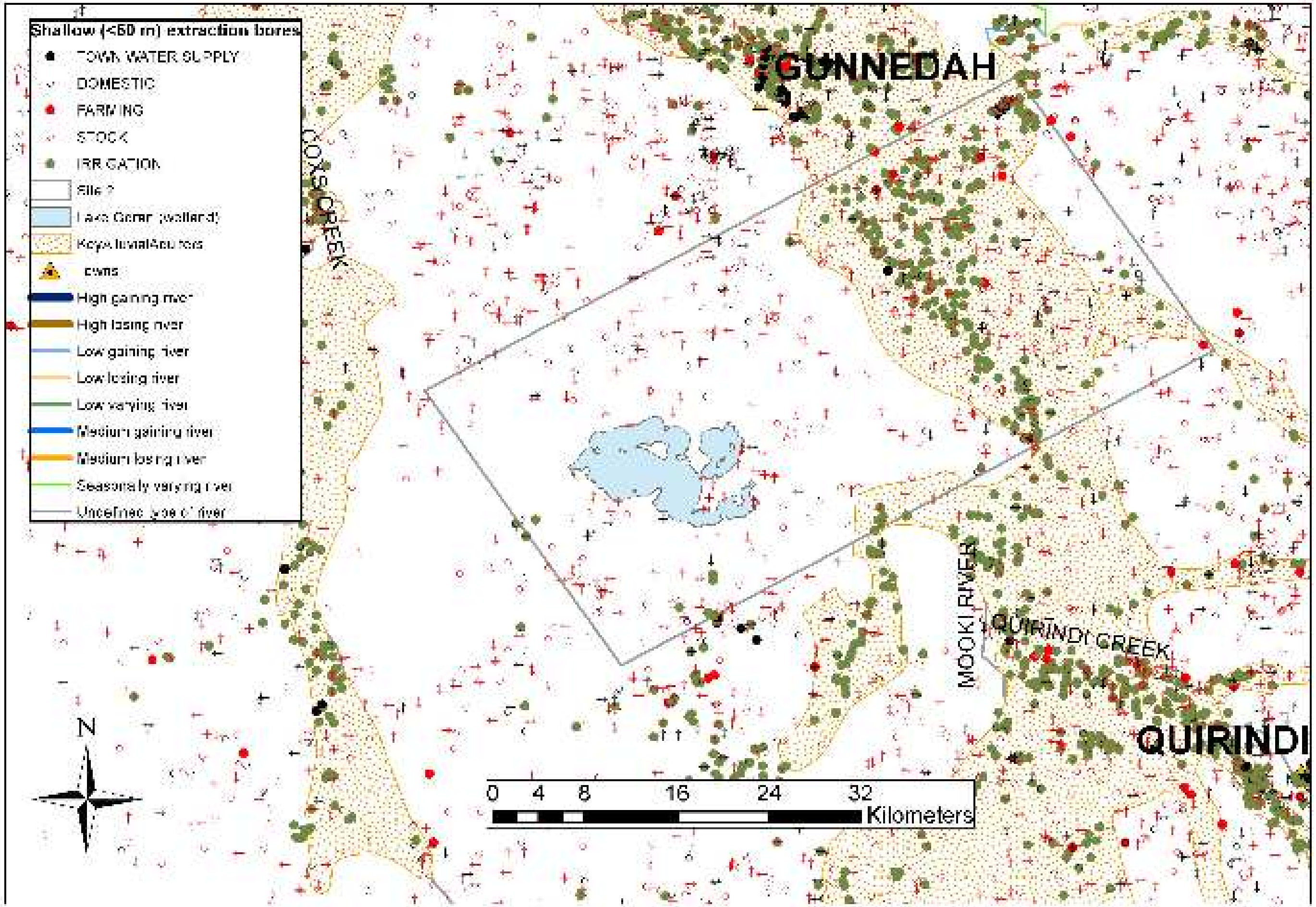
Wetlands

Exposure pathway is via contact with surface water within wetlands. The wetlands can be connected to rivers (valley bottom wetlands) or can be isolated (depression wetlands), depending on their location in the landscape. For valley bottom wetlands, the degree of connectivity with the groundwater and rivers can differ considerably. To maximise the impact, fully connected groundwater-wetland systems will be considered. High end concentrations in wetlands can then be obtained by assuming they are equal to concentrations in groundwater (no further dilution within the wetland is considered). Two cases are further discussed: wetlands connected to rivers and wetlands disconnected from rivers.



Source: BOM (2014)

Figure 5.15 Location of receiving environments in local Area 1, including shallow groundwater wells (< 50 m) and gaining Namoi River

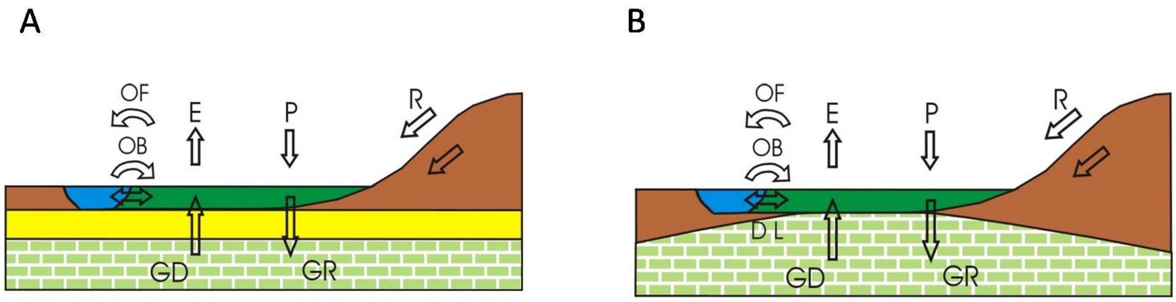


Source: BOM (2014)

Figure 5.16 Location of receiving environments in local Area 2, including shallow groundwater wells (< 50 m) and Lake Goran Wetland

Wetlands connected to rivers

Wetlands exchange water and chemicals with rivers. This can be in the form of input (from river to wetland) or output (from wetland to river) (Figure 5.17). The wetland is assumed to be connected to groundwater, and the maximum groundwater concentration in the layer underneath the wetland will be used. It is further assumed that only output of water and chemicals from wetland to river occurs, at a rate equal to the input from groundwater (water and chemicals). In this way no accumulation of chemicals occurs within the wetland.

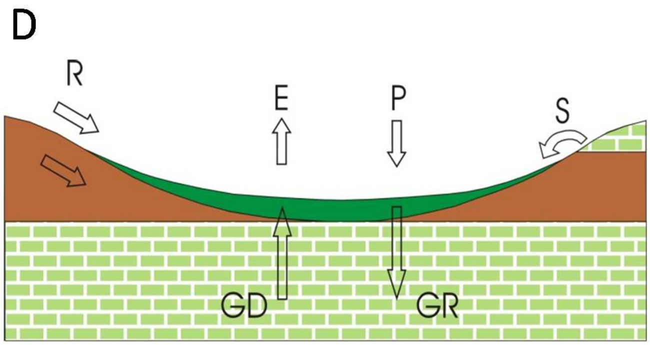


Source: Ramsar (2005). GD = groundwater discharge; GR = groundwater recharge; E = evapotranspiration; P = precipitation; R = runoff; OF = overland outflow; OB = overbank flow; D = drainage; L = lateral inflow.

Figure 5.17 Valley bottom wetland mainly fed by surface water–disconnected stream (A); Valley bottom wetland fed by surface water and groundwater–connected stream (B)

Wetlands disconnected from rivers

Wetlands receive contaminants by direct discharge from shallow groundwater (Figure 5.18). High end concentrations in wetlands can be obtained by assuming they are equal to the concentration in the shallowest groundwater (model) layer. Since there is no connection with rivers, the inflowing chemicals accumulate over time within the wetland.



Source: Ramsar (2005). For other fluxes see Figure 5.17

Figure 5.18 Depression wetlands fed by groundwater (D). S = spring flow

Springs

Exposure pathway is via contact with spring water. If springs have been identified in the area of interest, concentrations will be assumed equal to concentration in discharging groundwater. Examples of springs include the mud-mound springs on the Liverpool Plains (Acworth and Timms 2003).

Environmental data

This section provides site-specific environmental data to support selection of one area for detailed groundwater flow and solute transport modelling, and the development of the conceptual groundwater model of the selected area.

There are a number of ecosystems that rely on surface expressions of groundwater (i.e. rivers, springs and wetlands). As shown in Figure 5.19 there are sections of river that are either losing or gaining or seasonally varying in river stage. This connectivity status represents the results from the CSIRO Murray-Darling Basin Sustainable Yields Project (CSIRO 2007). Since then, the nature of connectivity may have been impacted by natural and anthropogenic factors such as wet/dry climate cycles, changes in groundwater supply for irrigation, and de-watering of mines recently becoming operational in the Narrabri vicinity. As a result, the 2007 status will likely have changed. Confirmation of such changes is beyond the scope of the current study.

According to the Namoi Catchment Management Authority Region there are currently 153 items in the Region listed under the NSW Threatened Species Conservation Act (NSW Government 2013) plus four species listed under the EPBC Act. Of the 153 NSW listings[15] there are: 86 vulnerable species, 27 endangered species, four critically endangered species, two endangered populations, and 16 endangered ecological communities. Within the Liverpool Plains CMA sub-region, there are 119 species, of which 37 are nationally listed species. The locations of endangered flora and fauna and groundwater dependent species are shown in Figure 5.20 and Figure 5.21, respectively.

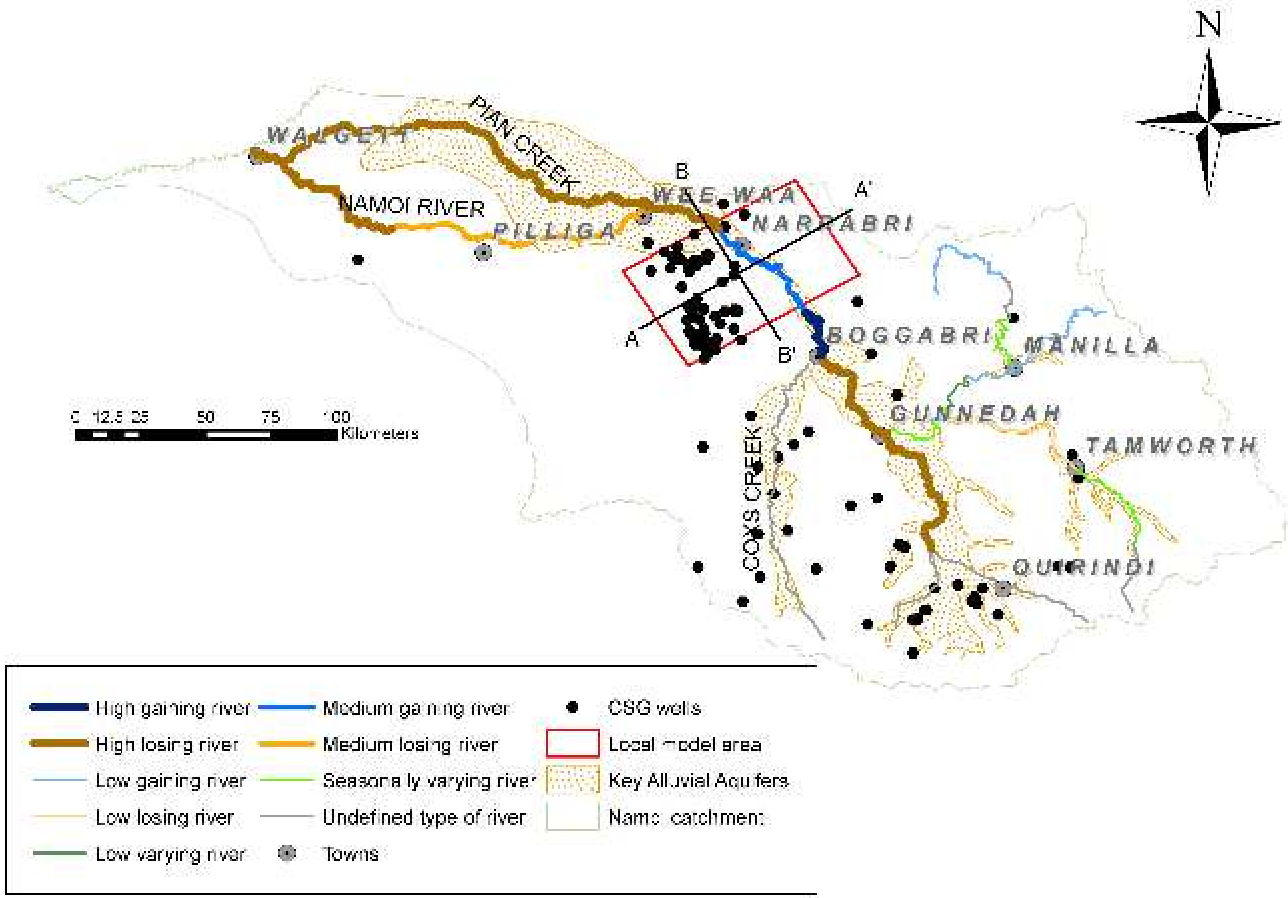
Similar to the exposure assessment for water wells, the number of endangered flora species and water dependent animal species within a given radial distance from a coal seam gas well can be spatially defined and quantified (Table 5.9).

Table 5.9 Number of endangered flora species and water dependent animal species at a given radial distance from the nearest coal seam gas well. Data applies to entire Namoi catchment

Radial distance from the nearest coal seam gas well (m)	Endangered flora species		Water dependent animal species	
	Number	Cumulative probability, %	Number	Cumulative probability, %
100	0	0	7	0.4
200	1	0.4	20	1.2
500	4	1.6	48	2.9
1000	11	4.5	205	12.4
2000	46	18.6	535	32.4
5000	104	42.1	1 056	63.9
10 000	247	100	1 652	100

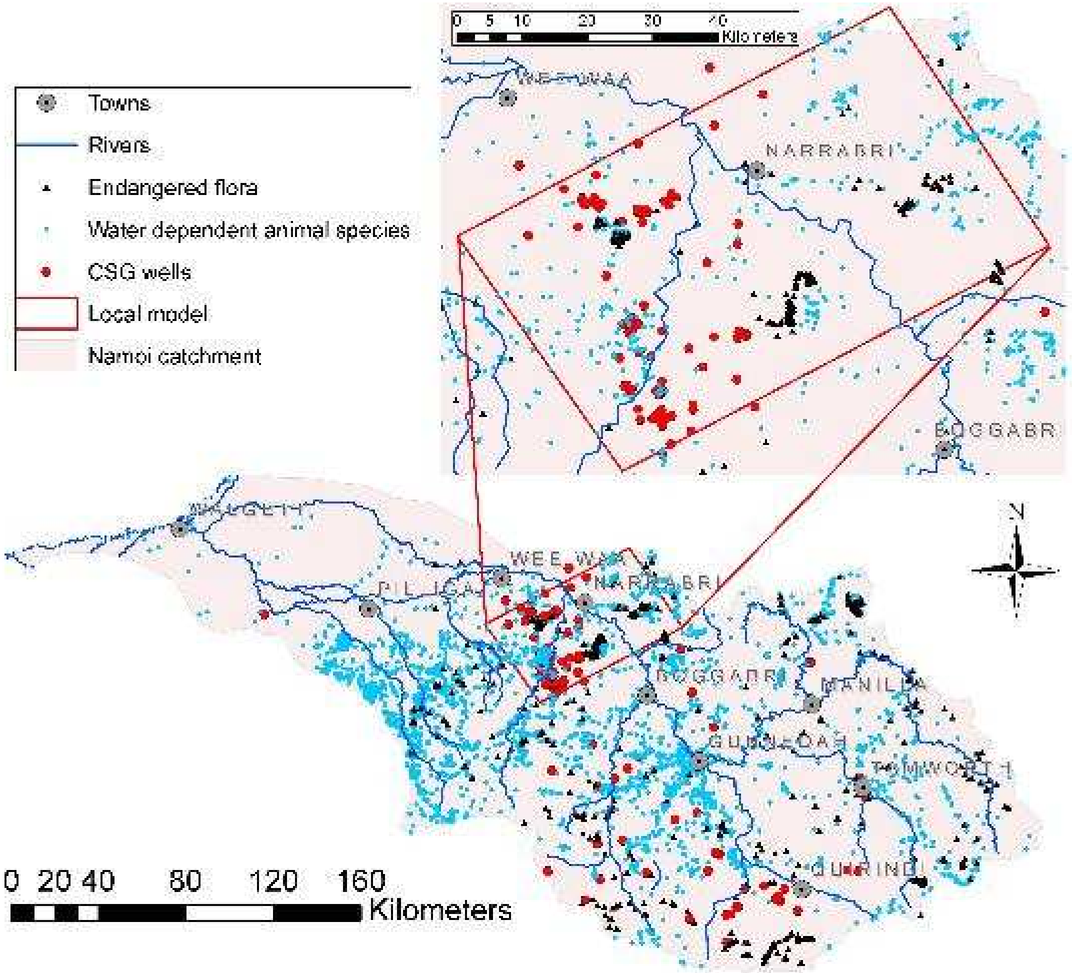
Source: NSW Government (2014b)

[15] For a complete listing see www.environment.nsw.gov.au/threatenedSpeciesApp/cmaSearchResults.aspx?CmaName=NamoiandSubCmaId=0



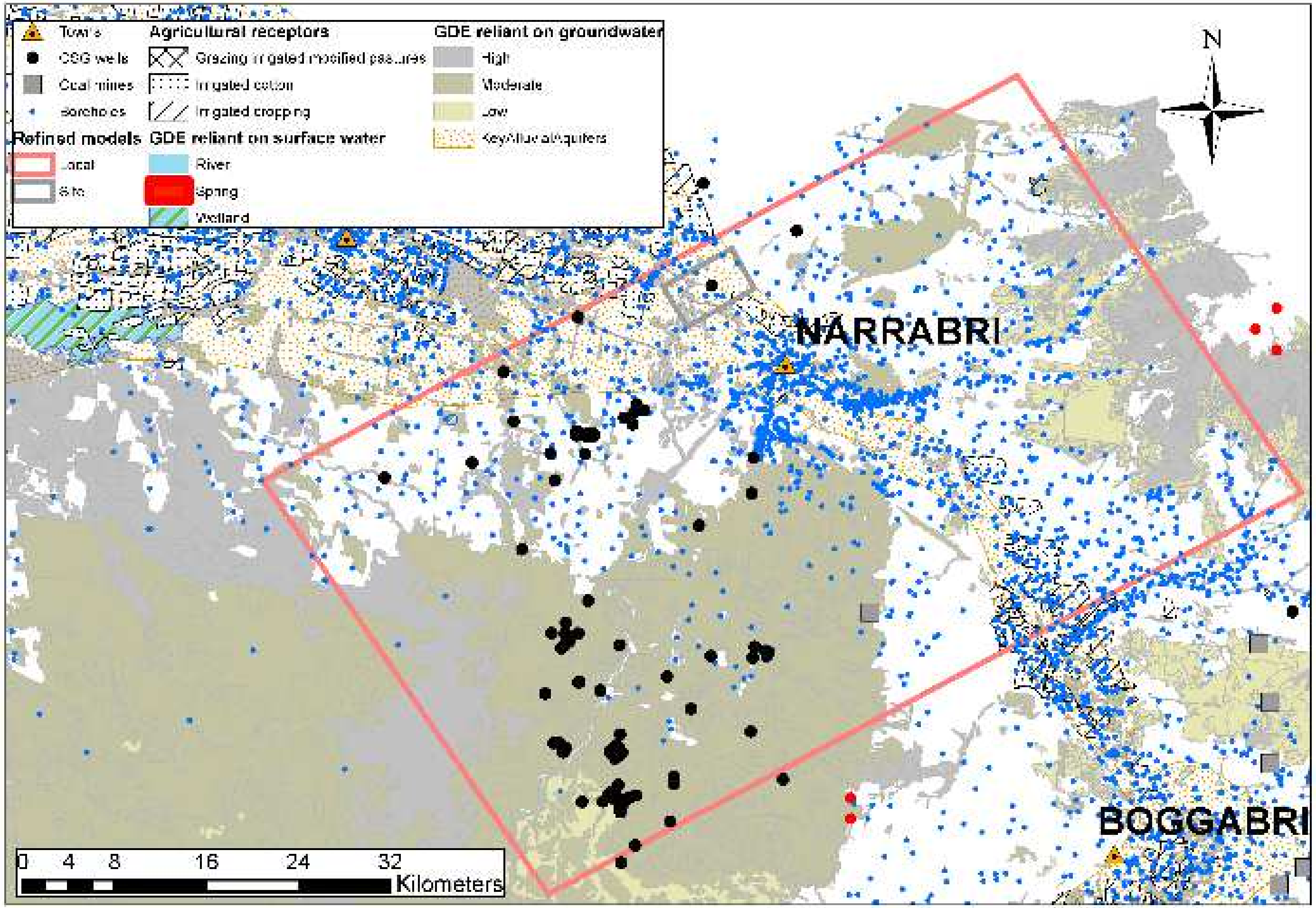
Data extracted from CSIRO (2007)

Figure 5.19 Rivers in the Namoi catchment and their hydraulic status (i.e. losing or gaining or seasonally varying)



Source: NSW Government (2014b)

Figure 5.20 Endangered flora and water dependent animal species in the Namoi catchment



Source: BOM (2013)

Figure 5.21 Groundwater dependent ecosystems that are reliant on surface water (e.g. rivers, springs and wetlands) and groundwater

It is again assumed for reasons of simplicity that the coal seam gas well is the location where the leak or spill occurs. This allows the expression, for the currently known locations of coal seam gas and water wells, of the likelihood of such species to be within a certain distance from a potential contamination source. This distance-likelihood function can be linked to the distance-consequence information obtained from the transport simulations (Mallants et al. 2017b). Vegetation types that rely on subsurface presence of groundwater are listed in Appendix B. The data considered applies to the entire Namoi catchment.

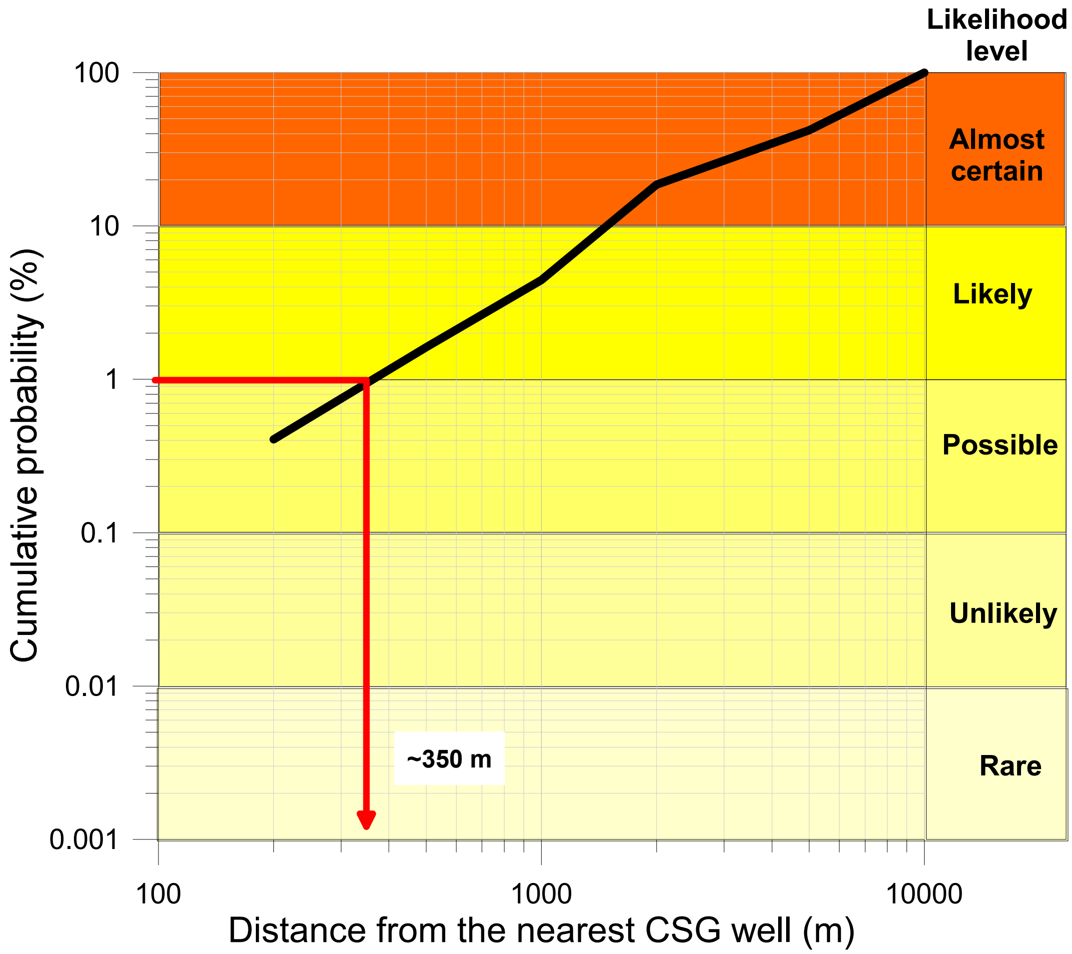
The corresponding empirical cumulative distribution functions of endangered flora species and water dependent animal species within a given distance from the nearest coal seam gas well are shown in Figure 5.22 and Figure 5.23. Note that only species within a distance of 10 000 m have been considered. The cumulative distribution reveals there is only a 1% chance of finding endangered flora species within a distance of approximately 350 m of a coal seam gas well, or conversely, in 99% of all cases endangered flora species will be at distances greater than approximately 350 m from a coal seam gas well. The closest distance reported between a coal seam gas well and an endangered flora species is 200 m. The probability that this occurs is only 0.4%, or 4 times out of 1 000. Details about the species for the 100 and 200 m distance class are given in Table 5.10.

Table 5.10 Endangered flora species (family name only) and water dependent animal species within 100 and 200 m of the nearest coal seam gas well

Radial distance from the nearest coal seam gas well (m)	Endangered flora species	Water dependent animal species (number of sites)
100	None	• Turquoise Parrot (3 sites) • Masked Owl (2 sites) • Grey-crowned Babbler (2 sites)
200	Poaceae (1 site)	• Grey-crowned Babbler (4 sites) • Speckled Warbler (4 sites) • Hooded Robin (1 site) • Koala (1 site) • Yellow-bellied Sheathtail-bat (1 site) • Pilliga Mouse (2 sites)

For water dependent animal species, the cumulative distribution reveals there is a 1% chance of finding such species within a distance of approximately 180 m of a coal seam gas well, or conversely, in 99% of all cases water dependent animal species will be at distances greater than approximately 180 m from a coal seam gas well. The closest distance reported between a coal seam gas well and a water dependent animal species is 100 m. The probability that this occurs is 0.4%, or 4 times out of 1 000. The fact that several bird species are involved in this data set complicates the analysis because of their migration ability. Nevertheless, it remains useful to have a first appraisal of the proximity of potential coal seam gas related contamination sources to habits of particular animal species. Details about the species for the 100 and 200 m distance class are given in Table 5.10.

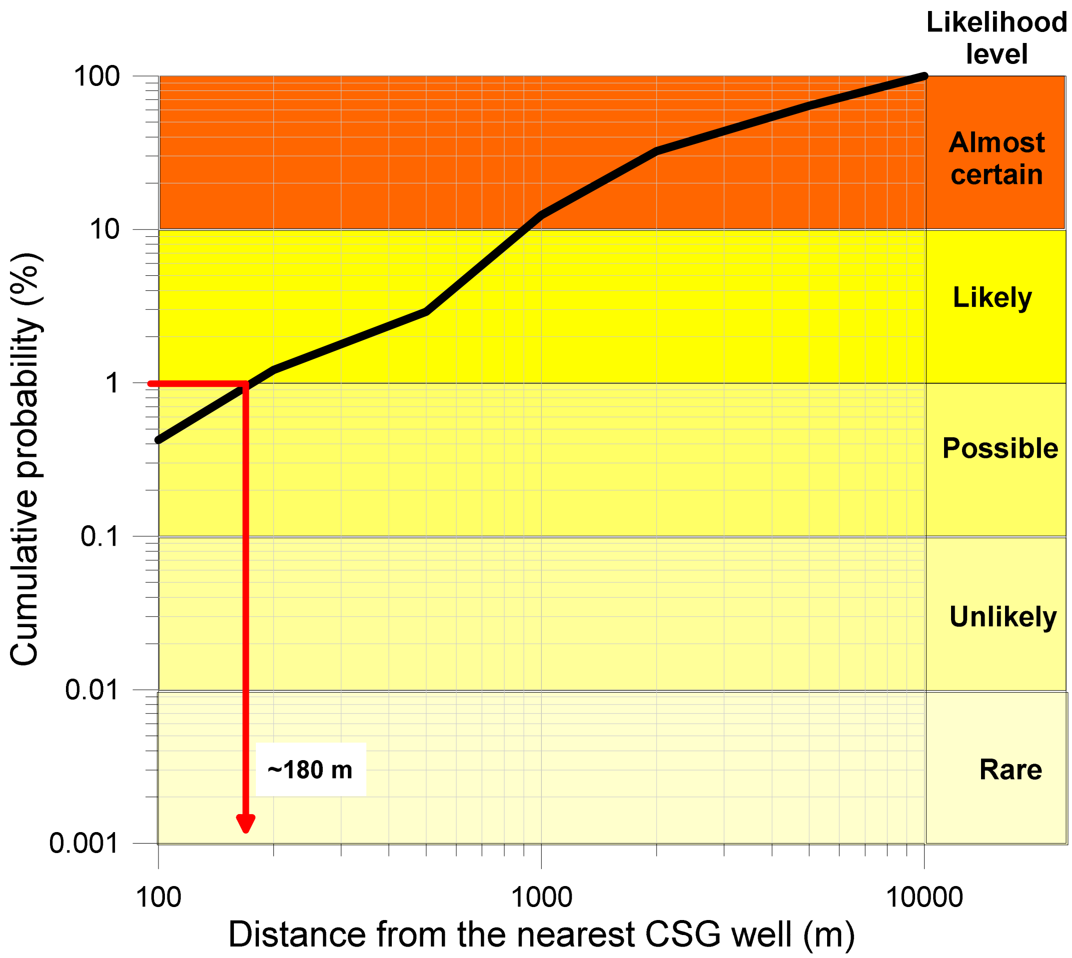
For future coal seam gas site developments, it is sufficient to calculate the distance to any of the existing receiving environments and apply this to the distance-likelihood relationship to quantify the probability of occurrence. The distance-likelihood relationship (Figure 5.22 and Figure 5.23) can also be used to define a buffer or exclusion zone around particular receiving environments which would help ensure a negligible probability of impact on particular species of fauna and flora.



Note. Likelihood levels can be used to develop a risk matrix (see Figure 2.2).

Figure 5.22 Empirical cumulative distribution of endangered flora species at a given distance from the nearest coal seam gas well

An analysis of the spatial proximity of springs (using the springs listed in Mallants et al. 2017a) to coal seam gas wells indicated zero springs were within a distance of 2 000 m, three springs were within a distance of 5 000 m, and an additional six springs were within a distance of 10 000 m. Thus, based on the underlying Namoi data, it will be highly unlikely to find any spring in the vicinity of chemical fate pathways associated with coal seam gas related surface activities (this relationship may not hold true in other bioregions where springs could, potentially, be more densely located). For this reason, springs will not be further considered in the conceptualisation and exposure calculations.



Note. Likelihood levels can be used to develop a risk matrix (see Figure 2.2).

Figure 5.23 Empirical cumulative distribution of water dependent animal species at a given distance from the nearest coal seam gas well

Several of the coal seam gas wells are located in areas that have been identified as providing the potential for ecosystems to be interacting with groundwater [for example, GDEs (BOM 2013)]. A total of eight coal seam gas wells are in areas where there is high potential for groundwater interaction, eight in areas with moderate groundwater interaction, and 14 wells in areas of low groundwater interaction.

5.3.3 Selection of area for modelling

In the previous sections two areas have been proposed for exposure assessments. One of the two was selected and will be developed into a groundwater model that is fit for detailed groundwater transport calculations. The two subregions have been selected in the vicinity of existing or planned coal seam gas developments, on the basis of providing sufficiently different hydrogeological features, and a wider variety of receiving environments. For example, the second area or local site was located in the upper part of the catchment and includes the iconic ecosystem of Lake Goran (see Section 5.3.2.4).

Both areas display contrasting interactions between groundwater and surface water: in Area 1 the main stream (the Namoi River) is considered to be a gaining stream while in Area 2 the stream (the Mooki River) is considered to be a losing stream (see Section 5.3.2.4). In Area 1 the groundwater and surface water are connected via discharging groundwater, indicating that the stream in this area has a much higher probability of receiving contaminated groundwater than Area 2, where such water connections probably do not exist.

The spatial dimensions in plain view for local Area 1 and Area 2 are 45 km by 67 km (a surface area of some 3 015 km^2) and 28 km by 53 km (surface area of 1 484 km^2), respectively. In the original Namoi Catchment Model a uniform 1 km^2 grid cell was used. The subregion area will have a higher spatial granularity to provide a better representation of groundwater flow velocities across the aquifer, proper representation of interfaces between groundwater and surface water, and to allow for a further grid refinement for the final transport simulation models whose grid cell dimensions are of the order of several tens of metres to limit numerical dispersion.

The selection of sub-domain areas was based on:

- potential risk based on ongoing and planned activities in regards to coal seam gas extraction
- sufficiently representative in terms of broad coverage of hydrogeological features
- sufficiently representative in terms of receiving environments of relevance to both human and environmental receptors.

On the basis of these criteria, the northern most area including the city of Narrabri has been selected for exposure assessment. This area has a larger number of coal seam gas wells (exploration, pilot and production wells) compared to Area 2. The potential likelihoods are, in theory at least, therefore higher in Area 1 than in Area 2.

With respect to hydrogeological representativeness, Area 1 contains a major stream (i.e. the Namoi River) with a considerable gaining section upstream of Narrabri to Cox Creek (Figure 5.19). The area contains the Gunnedah Formation (up to 115 m thick) which consists predominantly of gravel and sand with minor clay beds. It is the primary aquifer used for irrigation in the region. For exposure assessments, this formation would potentially yield significant hydraulic connections between the coal seam gas areas and receptor areas. This means that actual fate pathways would exist with relatively rapid transport of chemicals. In the alluvial area, depth to groundwater covers a broad range from 0 to 30 m.

Area 1 contains all relevant receiving environments, including shallow groundwater and shallow water wells in the alluvial aquifer, groundwater dependent wetlands, and a gaining river section. Among the shallow water wells, a much larger percentage are within short distances from coal seam gas wells compared to Area 2 (Table 5.8). Along the river, Area 1 has a much greater presence of wetlands mapped during the wetlands assessment and prioritisation project than Area 2 (Welsh et al. 2014).

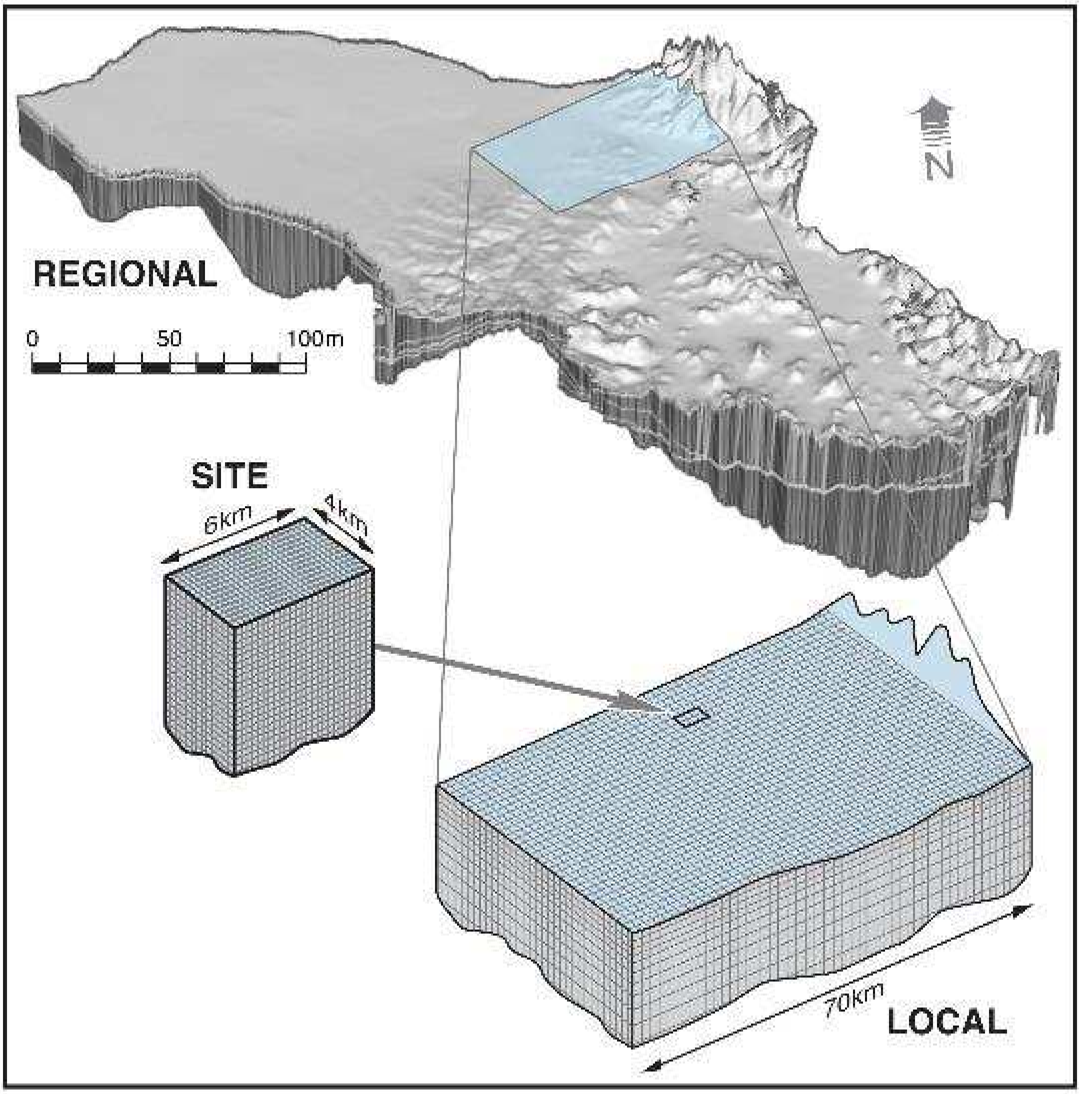
5.3.4 Model domain and geometry

Solute transport calculations require a fine spatial discretisation for reasons of numerical accuracy and stability. A very fine numerical grid (small elements or cells) can only be executed efficiently for a small numerical domain. An approach was developed to generate such a small domain (the site model) with a fine grid (delivering high spatial resolution). This means that, under a Tier 1 assessment, only a fraction of the existing coal seam gas sites are evaluated as only a limited number of small site domains are considered (here only one). Under certain circumstances (for example, site includes most receiving environments and / or hydrogeological features relevant to the chemical fate pathway) one area may suffice for exposure assessments. Additional model domains may be generated to evaluate other sites if the Tier 1 assessment demonstrates that for certain chemicals the impact is not negligible. The subsequent discussion focuses on:

- the need for solute transport models with fine spatial discretisation
- the location and characteristics of local models from which the very detailed site model will be developed
- the numerical procedure(s) to generate such high-resolution grids
- the hydrostratigraphic cross-sections for the two local models
- a conceptual representation of the site model.

One of the challenges of modelling the large dimensions of a catchment is the excessive requirement for data and computational resources (CPU time). A coarse grid for a large scale model is advantageous in terms of CPU time. However, the large grid cells would generate large water balance errors; would not be able to represent important hydrogeological features, contaminant sources, large concentration gradients, and receiving environments at a sufficiently detailed spatial resolution; and would also not be suitable for solute transport calculations where small grid cells are a pre-requisite for reducing numerical dispersion and oscillations. On the other hand, large scale models are useful to provide estimates of the groundwater balance at a regional scale, and their groundwater levels and fluxes can be used in developing more detailed local models. This can be better calculated where the regional groundwater model levels and fluxes become useful boundary conditions and natural groundwater boundaries such as streams and divides are not available. Such hierarchy of nested models is depicted in Figure 5.24. Several variants of such nested models exist, for instance with several different site models developed from a single local model.

Within Area 1, three smaller scale site models with a finer discretisation than the local groundwater flow model are initially considered for solute transport calculations; Figure 5.25 shows the example for local model 1. Only Site Model 3 was developed in a flow and transport model at this stage (Mallants et al. 2017b). The fine sub-grid transport models are essentially nested within the local groundwater flow model. A finer discretisation offers the advantages of enabling the user to accurately delineate the contaminant source area and the target receiving environments, while minimising numerical dispersion and oscillations (Gedeon and Mallants 2012). The principle of nested models was used in this study, with one local model being developed from an existing regional groundwater model, and this local model having at least one site model (the local model currently had three potential site models, see Figure 5.25). The groundwater head distribution obtained from the local groundwater model was then used to define the initial and boundary conditions for the site model such that reliable solute transport calculations could be performed.

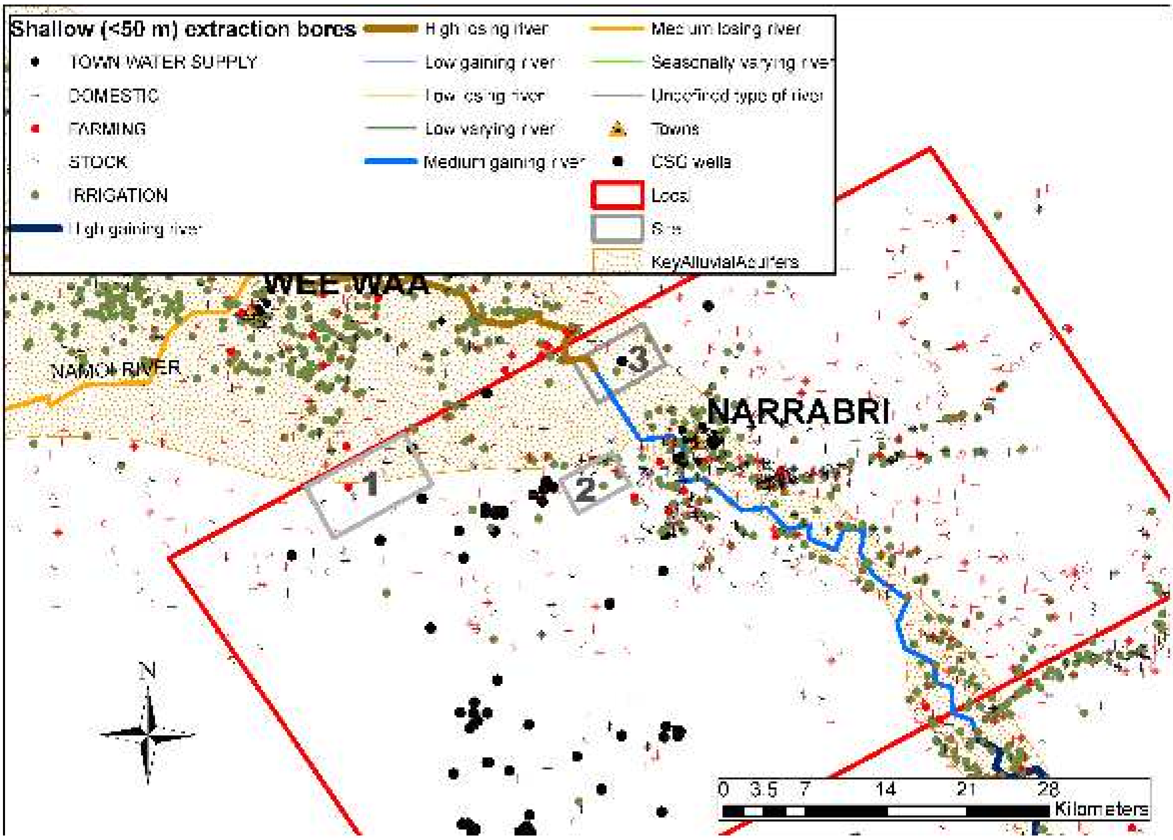


Note: Regional model is the Namoi Catchment Model developed by Schlumberger Water Services Ltd (SWS 2012a).

Figure 5.24 Developing a detailed small-scale site model for solute transport within a local model using a series of nested models based on the local grid refinement (LGR) method

Several procedures exist in MODFLOW for developing subsequent grid refinements, including techniques such as:

- telescopic mesh refinement (TMR; Leake and Claar 1999)
- local grid refinement (LGR; Mehl and Hill 2005)
- refinement of an unstructured finite volume mesh (USG; Panday et al. 2013).

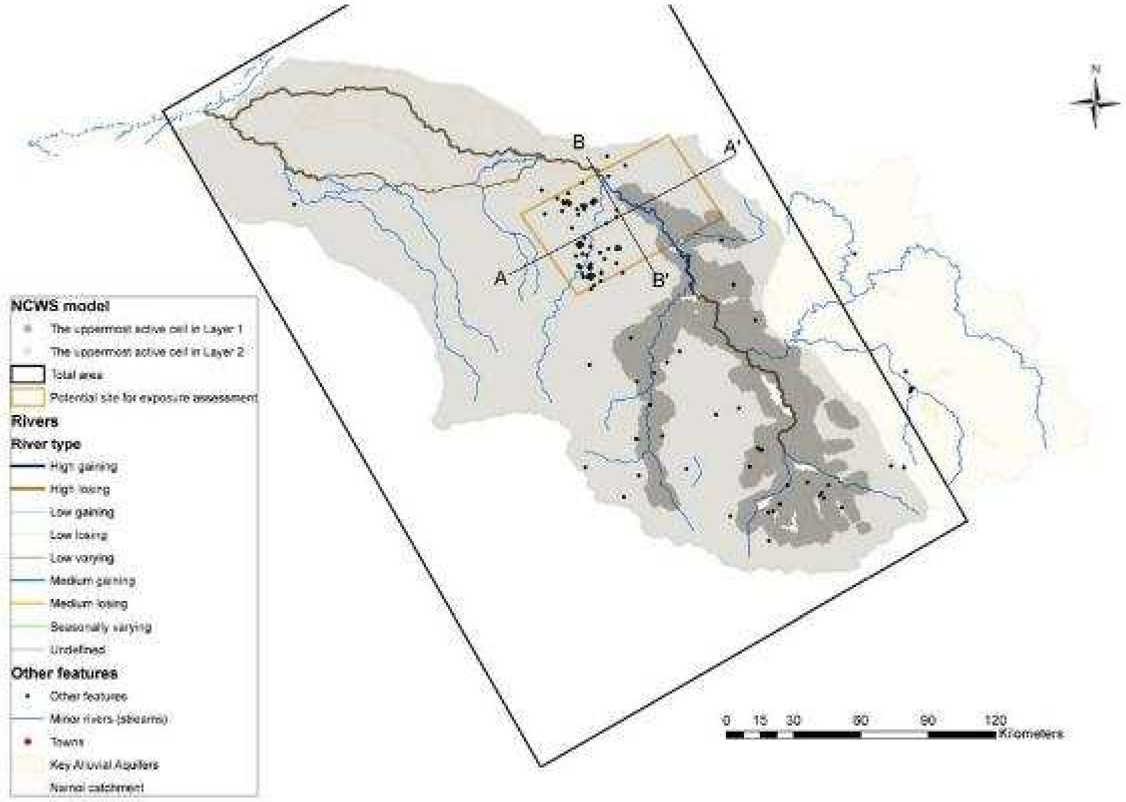


Source: BOM (2014).

Figure 5.25 Location of three potential site models within the local model 1

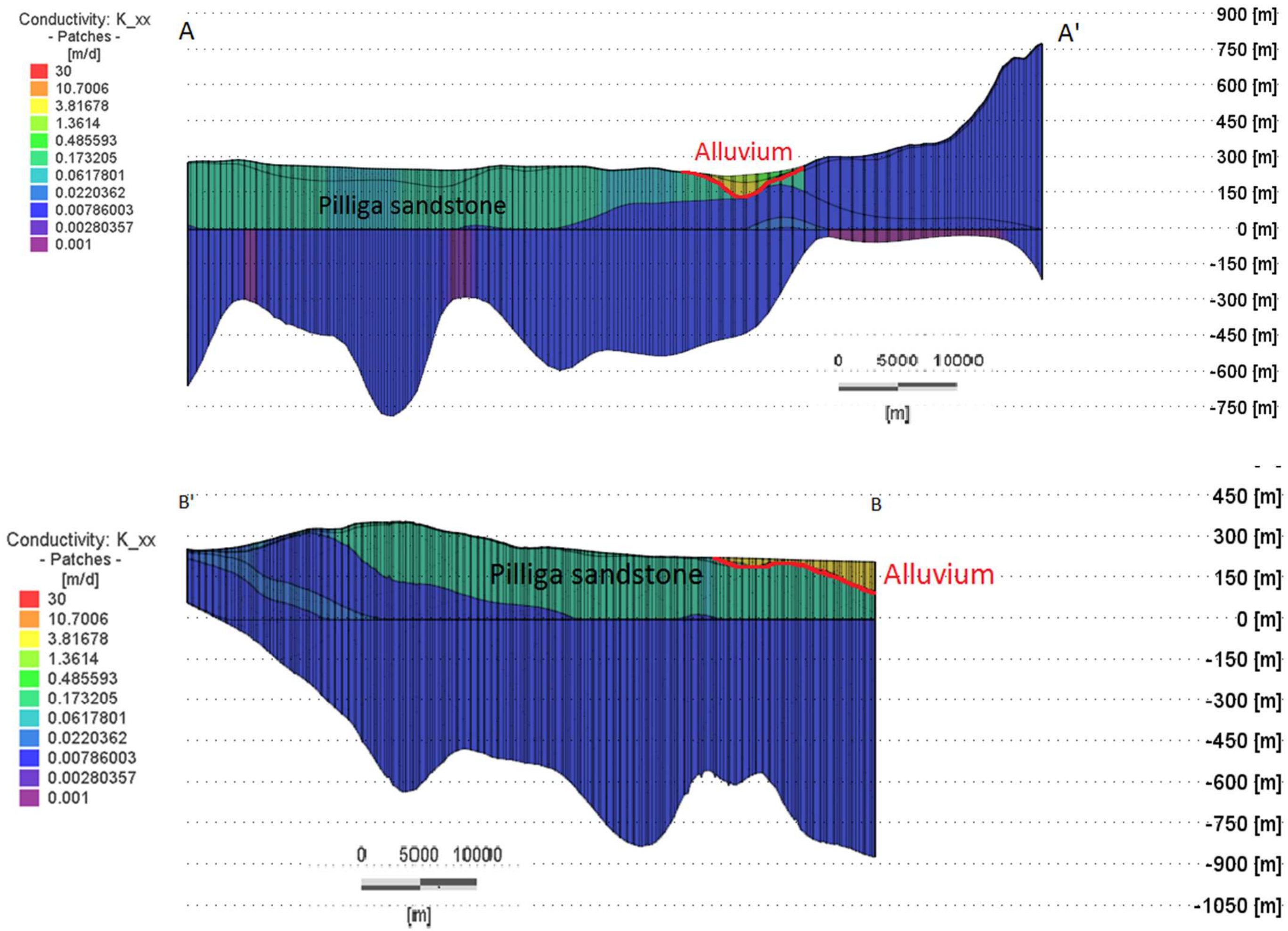
For the current exposure assessment, the coarser regional model grid and the nested local and site sub-grids will be coupled by using the LGR method. The grid resolution can be increased vertically as well as horizontally. This method links a coarse grid covering a large area, which incorporates regional boundary conditions, and a fine grid, covering a smaller area of interest. Two-way iterative coupling with shared nodes or ghost-nodes is used to ensure that the heads and fluxes are consistent between the two grids to obtain accurate solutions. Another option is traditional one-way coupling of either heads or fluxes, which does not resolve inconsistencies in heads and fluxes across the interface between two model grids. As demonstrated in a case study by Gedeon and Mallants (2012), the LGR method can produce smoother coupling heads with a smaller flux error at the interface between the coupled grids and requires less computational time than the one-way coupled method (TMR). However, the LGR method does not support multiple levels of refinement. That is, in order to produce small-scale site models used for transport calculations, the local LGR models will have to be decoupled from the regional model and repeated as stand-alone models, into which subsequently the refined site models are nested. These groundwater flow site models will then allow extracting groundwater velocities needed to establish the link to MT3D or MT3DMS (Zheng and Wang 1999) for solute transport model runs.

Figure 5.26 depicts the location of the selected subregion Area 1 with cross-sections of the hydrostratigraphic layers shown in Figure 5.27. Although the description of the numerical model is beyond the scope of the current report, the numerical model allows for schematised representation of the geological layers.



Data source: BOM (2014), Model source: SWS (2012b). Shaded areas pertain to the extent of the two uppermost layers conceptualised in the regional Namoi Catchment groundwater model.

Figure 5.26 Location of subregion Area 1 showing lines of cross-sectional views (AA', BB') of simplified hydrostratigraphy (see Figure 5.27)

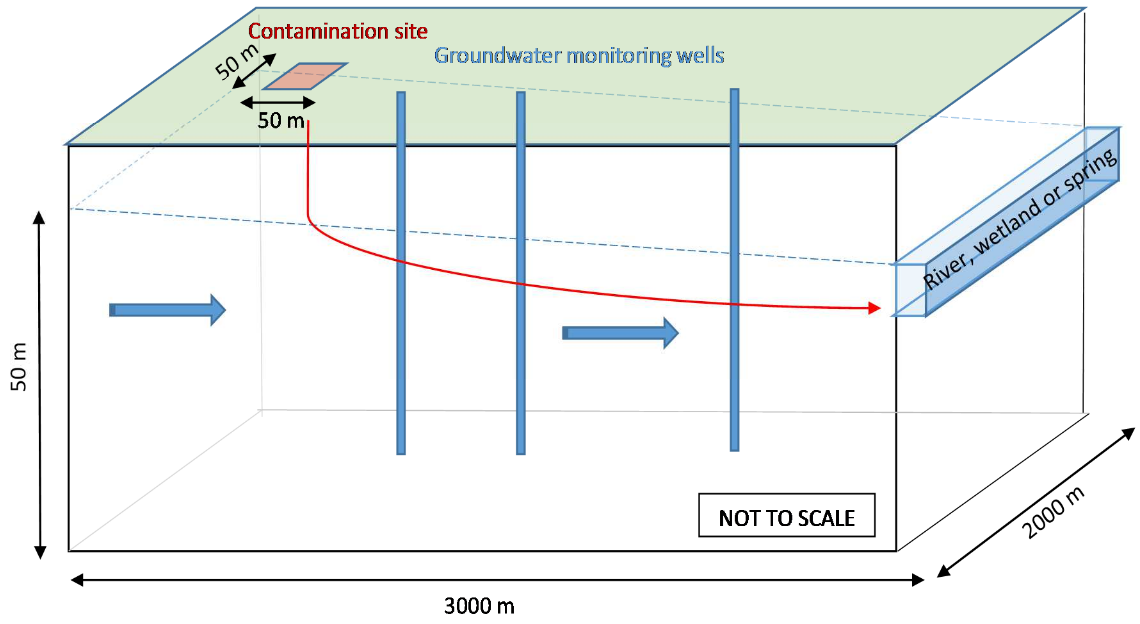


Extracted from SWS Namoi Catchment groundwater model, SWS (2012b)

Figure 5.27 Cross-sections AA' and BB' of simplified hydrostratigraphic layers for local Model 1 shown in Figure 5.26

The alluvial aquifers occupy 7 334 km^2 or 17% out the total catchment area of 42 064 km^2. Whilst the alluvial aquifers represent a small fraction of the total groundwater model, they are the areas with the highest density of wells (Section 5.3.2.3) and as such the likelihood for wells intercepting a contaminant plume that would originate from a nearby coal seam gas site would also be high.

A schematic representation of a site model used for transport calculations is given in Figure 5.28. One such site model will be inserted into the local model according to the principle shown in Figure 5.24 and for a location given in Figure 5.25, thereby applying grid refinement. There can be one or several receiving environments incorporated in the model, depending on whether a small model domain can encompass more than one receiving environment as they exist in the real landscape.

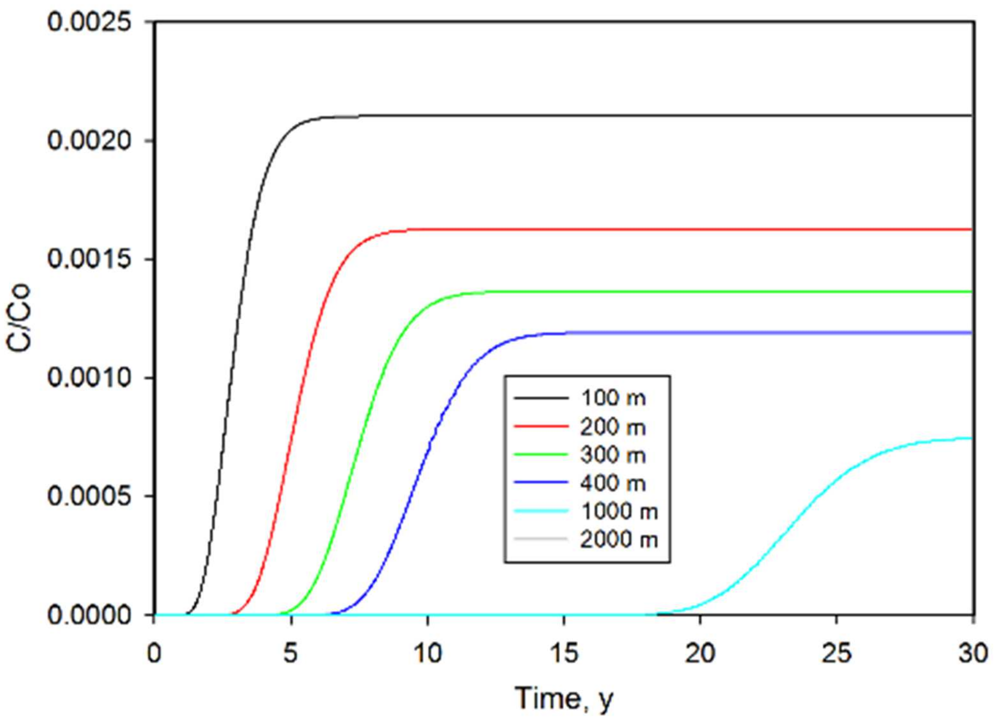


Receiving environments shown include water wells and a river or wetland.

Figure 5.28 Conceptual diagram of a site model used for solute transport calculations. Dimensions are not to scale.

The single conceptual model shown in Figure 5.28 will be run multiple times using parameter combinations based on the local model's parameter distributions (see Section 5.3.6) such that the regional model's groundwater velocity distributions are more or less replicated. The multiple runs generate multiple sets of dilution factors that will be summarised in lookup tables (see Table 5.6).

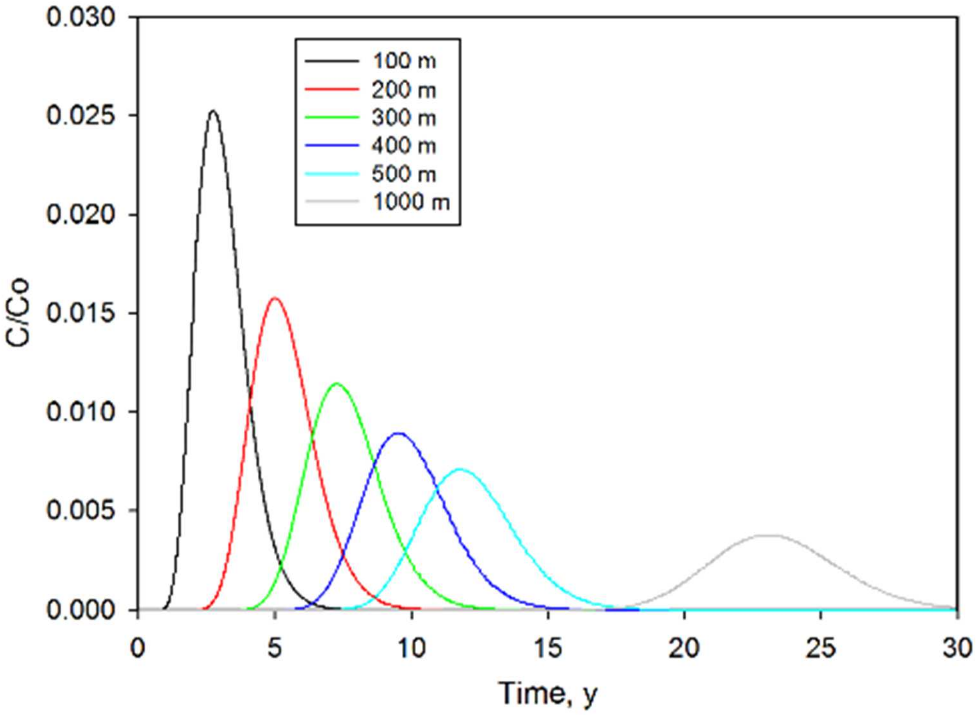
For the purposes of illustration, two examples are shown. The first considers continuous solute release during a period of 30 years (Figure 5.29). Breakthrough curves are shown at five different groundwater wells whose distance to the sources ranges from 100 to 2 000 m. As the distance from the solute source increases, the maximum concentration in the well decreases. At a distance of 100 m the initial source concentration of 1 unit has decreased to slightly above 0.002 (a dilution factor of nearly 500). At 1 000 m from the source the maximum concentration is between 0.001 and 0.0005 (or a dilution factor between 1 000 and 2 000).



Note. Continuous pulse for 30 years (hydraulic gradient = 0.001 m/m, K_H = 30 m/d, K_V = 0.3 m/d, effective porosity = 0.25). Longitudinal dispersivity = 5 m, horizontal transverse dispersivity = 0.5 m, vertical transverse dispersivity = 0.5 m. Infiltration rate = 0.033 m/year; total infiltrated volume of solute = 1×50×50 m^3.

Figure 5.29 Calculated relative concentration (C/C_0) at groundwater wells with increasing distance from the solute source

The second example is for a pulse application using the same flow and transport parameters as in the first example (Figure 5.30). Breakthrough curves now show a typical bell-shaped behaviour with the maximum concentration decreasing rapidly as transport distance increases. The maximum concentration is higher than in the previous case (Figure 5.29) owing to the injection of the same volume of solute during a much shorter period (4 days rather than 30 years). In other words, the same mass of chemical is added to the groundwater but during a much shorter period; hence there is less opportunity for dilution in space and time.



Solute pulse boundary condition with source duration = 4 days (hydraulic gradient = 0.001 m/m, K_H = 30 m/d, K_V = 0.3 m/d, effective porosity = 0.25 m^3/m^3). Infiltration rate = 0.25 m/day; total infiltrated volume of solute = 1×50×50 m^3.

Figure 5.30 Calculated relative concentration (C/C_0) at groundwater wells with increasing distance from the solute source

5.3.5 Initial and boundary conditions for the reference scenario (including interfaces with soil pathway)

Initial and boundary conditions need to be specified for groundwater flow and solute transport calculations. The groundwater flow model considers both inflow and outflow processes. The groundwater inflow processes in the local models include diffuse recharge as well as losses from rivers and streams (MODFLOW River package). The groundwater outflow processes consist of background extraction, such as for irrigation, stock and domestic, public supply and industry (Multi-Node Well package), coal seam gas wells (Multi-Node Well package), coal mine depressurisation (Drain package) as well as river and stream gains (River package). Evaporation is not explicitly defined in the groundwater model.

River stages are the same in each stress period. The stages vary in Model 1 from an all-time maximum 270.8 m upstream to an all-time minimum of 198.6 m downstream. In Model 2 they vary from an all-time maximum 283.7 m to an all-time minimum 263.6 m, respectively.

The detailed site model for solute transport simulation needs a proper solute boundary condition at the interface between the unsaturated zone and groundwatertable. To designate a contaminant source in the model requires either assigning constant concentrations to grid cells at the interface or assigning the same grid cells as point sources with an accompanying water flux rate. The solute boundary condition cells can be time-invariant or time-varying concentration cells. Both cases are applicable in situations where the source represents leakage from a produced water storage pond that has either a constant or varying solute concentrations over time.

5.3.6 Processes and parameters

This section provides further details on the hydrogeological properties within the regional and local models for the reference scenario and for the additional calculation cases that consider parameter perturbations of the reference parameters. The main focus of this study is on exposure pathways within shallow alluvial aquifers; however, there are parts of the catchment where there are deeper layers such as where the Pilliga Sandstone outcrops at the ground surface, as shown in Figure 5.27. Because coal seam gas exploration wells exist within the Pilliga Sandstone, an assessment needs to be made if results obtained from the alluvial aquifers can be used as a reasonable substitute for the Pilliga Sandstone (see Mallants et al. 2017b).

5.3.6.1 Groundwater flow for the reference scenario

A summary of important hydrogeological parameters (horizontal (K_H) and vertical (K_V) hydraulic conductivity, specific yield (S_Y), specific storage (S_S), and Darcy groundwater velocity (q_D)) was extracted from the full Namoi Catchment Model and for the local Model 1 and 2 derived from the full model. Values for these parameters for all 21 numerical layers for the full Namoi Catchment Model are available in Appendix A (Table A1). These values are different from those listed in Table 4.6 (SWS 2012a, 2012b). The difference is due to unreported additional calibration of the NCM that was not reported in the main SWS study. Given the nature of the regionalised generic models and the high end exposure assessment predictions reported here, the quality of calibration is much less of an issue than it would be for a site specific analysis. Moreover, the approach adopted here considers, in addition to the reference model run, the running of the models with different combinations of hydrogeological parameters to generate outputs that are representative of a wider area than just that of the detailed site model.

For the full model, the minimum, maximum, and arithmetic mean for horizontal (K_H) and vertical (K_V) hydraulic conductivity, specific yield (S_Y), and specific storage (S_S) are provided in Table 5.11 for the most relevant layers in this study. These parameter ranges can be considered as currently the best available hydrogeological data for the Namoi catchment and thus form the basis for the reference scenario.

Table 5.11 Hydrogeological parameters for the full regional model as considered in this study

Layer #	Geological equivalent (unconfined)	Horizontal conductivity (m/day)			Vertical conductivity (m/day)			Specific yield (-)			Specific storage (m^{-1})		
		min	max	mean	min	max	mean	min	max	mean	min	max	mean
1	Narrabri	10^{-3}	3×10^{1}	5×10^{0}	5×10^{-5}	5×10^{-1}	1.8×10^{-1}	5×10^{-3}	2.5×10^{-1}	6×10^{-2}	10^{-6}	5×10^{-4}	1.6×10^{-4}
2	Gunnedah	10^{-3}	10^{-1}	6×10^{-2}	10^{-5}	10^{-3}	10^{-4}	10^{-2}	10^{-1}	7×10^{-2}	10^{-6}	10^{-5}	7×10^{-6}
3	Lower Namoi Alluvium/ weathered horizon	10^{-3}	10^{-1}	6×10^{-2}	10^{-5}	10^{-3}	9.5×10^{-4}	10^{-2}	10^{-1}	7×10^{-2}	10^{-6}	10^{-5}	7×10^{-6}
4	Fractured rock horizon	10^{-3}	10^{-1}	5×10^{-2}	10^{-5}	10^{-3}	1.5×10^{-4}	10^{-2}	10^{-1}	2×10^{-2}	10^{-6}	5×10^{-6}	5×10^{-6}
5	Great Artesian Basin	10^{-3}	5×10^{-2}	4×10^{-2}	10^{-5}	10^{-3}	1.5×10^{-4}	10^{-2}	10^{-1}	3×10^{-2}	10^{-6}	5×10^{-6}	5×10^{-6}
6	Pilliga sandstone	10^{-3}	5×10^{-2}	10^{-2}	10^{-5}	10^{-3}	1.5×10^{-4}	10^{-2}	10^{-1}	9×10^{-2}	10^{-6}	5×10^{-6}	5×10^{-6}

Data in Table 5.12 allows a comparison between groundwater velocities derived from the regional model and the local Model 1 and 2 for the first two model layers (Narrabri and Gunnedah). In this way, an assessment is made of how representative the sub-models are in regard to capturing the variation in groundwater velocities in the much larger regional model. Note that for solute transport calculations, groundwater velocities (*q*) will be converted in the solute transport model into pore water velocities (*v*) by dividing *q* by the effective porosity (n_e). The pore water velocity is the rate at which chemicals migrate through the aquifer; it defines the travel time of a chemical from a source to a receptor.

Table 5.12 Groundwater (Darcy) velocities (m/d) for a single realisation of the full regional model and local Model 1 and 2

	Model 1		**Model 2**		**Regional model**	
	Layer 1 Narrabri	**Layer 2 Gunnedah**	**Layer 1 Narrabri**	**Layer 2 Gunnedah**	**Layer 1 Narrabri**	**Layer 2 Gunnedah**
Minimum	2.05×10^{-6}	2.05×10^{-6}	2.05×10^{-6}	2.05×10^{-6}	2.05×10^{-6}	2.60×10^{-7}
Maximum	1.77×10^{-1}	8.03×10^{-2}	7.55×10^{-1}	4.72×10^{-2}	9.77×10^{0}	4.01×10^{-1}
1st Quartile	1.28×10^{-3}	2.05×10^{-6}	1.64×10^{-3}	2.51×10^{-5}	3.10×10^{-3}	2.40×10^{-5}
Median	2.69×10^{-3}	3.55×10^{-5}	2.95×10^{-3}	2.60×10^{-4}	1.50×10^{-2}	1.90×10^{-4}
3rd Quartile	1.77×10^{-2}	2.29×10^{-3}	7.78×10^{-3}	5.29×10^{-3}	1.88×10^{-1}	1.96×10^{-3}

Prior to the solute transport simulations, groundwater flow simulations need to be carried out using MODFLOW. The groundwater velocities thus obtained will be used in the subsequent transport simulations with MT3DMS.

5.3.6.2 Groundwater flow with perturbed parameters

To allow for evaluation of a broader range of groundwater flow conditions, different combinations of hydrogeological parameters were considered. Horizontal hydraulic conductivity (K_H) was perturbed for the higher resolution site model (see Figure 5.24) in the following way: all conductivity values were increased and decreased by a factor of 5. In this way a sufficiently broad range in conductivity values is evaluated. The vertical anisotropy in hydraulic conductivity (K_H/K_V) was not changed. The hydraulic gradient was varied by modifying the river bed conductance reference value by a factor of 7; in other words using conductance values seven times smaller and seven times larger than the reference value (for details, see Mallants et al. 2017b).

5.3.6.3 Solute transport

The conceptual model for solute transport simulations is depicted in Figure 5.28. As the focus of the study is on impacts on shallow groundwater, the uppermost layers corresponding to the alluvial aquifers (Layers 1 and 2) are considered only. Multiple runs were envisaged using groundwater velocities generated with the detailed groundwater flow model (site model 3 from Figure 5.25). These calculations were carried out with hypothetical solute concentrations at the source area (i.e. at the groundwatertable) and have been reported in Mallants et al. (2017b). Dilution factors in groundwater were calculated independently from those of the unsaturated zone (for details, see Mallants et al. 2017b).

The groundwater flow calculations are based on perturbations of the hydraulic conductivity (low = reference value / 5, reference, high = reference value x 5) and the river bed conductance (low = reference river conductance / 7, reference, high = reference river conductance x 7), thus producing nine groundwater flow runs for subsequent transport calculations. The solute transport simulations will further consider perturbations of the effective porosity, with again three values: 0.10, 0.20 (reference), and 0.40. This range in porosity corresponds more or less to the range of reported values from 0.15 to 0.39 (see Section 4.3). As a result, 27 solute transport simulations were carried out for the detailed site model (Mallants et al. 2017b).

At this stage of the exposure assessment, the only transport processes accounted for are advection (transport as a result of flowing water) and hydrodynamic dispersion. Hydrodynamic dispersion (mechanical dispersion and molecular diffusion) can be introduced either by assigning physical dispersion in the solute transport equation or it can be generated automatically due to numerical dispersion[16].

5.3.6.4 Time frames for exposure assessment

The main coal seam gas activities within a well field may typically last for 20 to 30 years, not including the 3 to 5-year baseline phase (site identification, access and preparation) and the return to hydraulic equilibrium phase (decommissioning, rehabilitation). While the likelihood of chemical emissions may be low, should coal seam gas chemicals be inadvertently released into the environment the impact will be noticeable (i.e. with measureable concentrations significantly different from baseline values) for a relatively long time as a result of relatively slow migration and attenuation in soil and groundwater; and / or in some cases, will become noticeable in groundwater monitoring wells only after much longer time periods (owing to the generally slow migration in the unsaturated soil prior to reaching groundwater). It is therefore important to consider impacts over an appropriate time frame to ensure chemical impacts (‘consequences’ in a risk assessment framework) are not underestimated. Some guiding principles for defining timeframes for quantitative chemical risks and environmental impact assessments include:

- Assessments should be able to quantify and predict the chemical peak, both in terms of concentration and over time. Hence, timeframes should be long enough to allow for the peak to occur within the different receiving environments and environmental compartments.
- Assessment timeframes must look beyond the operational injection and depressurisation phases of a coal seam gas well field. This means that assessments will need to consider potential cumulative impacts over 50 to 100 years or more.
- There are considerable uncertainties associated with long-term assessments. It is thus useful in this regard to refer to international guidelines, e.g. those related to management of radioactive waste. For instance, no cut-off time is considered in IAEA/EU (2003a, 2008a) guidelines. There is a need to calculate maximum impact, but if it is predicted beyond a generational timeframe then it can only be of practical use if presented in a qualitative way.

[16] An error term resulting from the finite difference solution of the solute transport equation.

6 Confidence building for impact assessment modelling

6.1 Introduction to confidence building in numerical simulation

The subsurface science and engineering community is providing robust assessments of risk and engineering performance for important issues with far-reaching consequences. Examples include long-term impact assessments of temporary or permanent waste disposal sites, contamination plumes in soil and groundwater, and resource mining with significant impacts on groundwater resources. As a result, the complexity and detail of subsurface processes, properties, and conditions that can be simulated has significantly expanded. This expansion is enabled, in part, by advances in measurement technology, computing technology, and numerical techniques. Independent data for validating these increasingly sophisticated predictions are not available and are unlikely to be available in the near future. Comparison of numerical simulators with closed form analytical solutions (i.e. mathematical expressions that are easily solvable using a finite number of well-known standard expressions) are necessary and useful but limited to situations that are far simpler than typical applications that combine many modelling options. The more successful benchmarking exercises are based on the cooperative involvement of multiple simulator teams. Successful large-scale benchmark initiatives include HYDROCOIN[17] (Larsson 1992), INTRAVAL[18] (Larsson 1992), and BIOMOVS[19] (Davis et al. 1999).

In addition to predictive calculations, impact assessments typically involve system descriptions (conceptual models) and supporting databases, scenario analyses, consequence analyses, sensitivity and uncertainty analyses, and a comparison of estimated impact to regulatory requirements. If different stakeholders are to have confidence in the results and conclusions drawn from impact assessments, and recognising that different stakeholders will have different needs, expectations, and concerns, it is important that key information is provided in a transparent and traceable manner, and that evidence is provided that the computer codes and conceptual models are fit for purpose and have been used appropriately (IAEA 2008b; Perko et al. 2009b).

Elements of confidence building in quantitative impact assessments include:

- rigorous record keeping and quality assurance procedures to ensure the calculations and results are those intended, and are fully traceable and reproducible
- scientific and technical understanding of the processes and events involved, i.e. justification of the information that is compiled in the assessment basis
- models, codes and data that are ensured through the verification, qualification and, when possible, validation process

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[17] HYDROCOIN (HYDROlogic Code Intercomparison) addressed code verification, model validation and sensitivity and uncertainty analyses of groundwater flow calculations.
[18] INTRAVAL (INternational TRAnsport model VALidation) advanced the state of knowledge on qualitative and quantitative methods to demonstrate the accuracy of geosphere transport codes.
[19] BIOMOVS (BIOspheric MOdel Validation Study) tested models designed to calculate the environmental transfer and bioaccumulation of radionuclides and other trace substances.

- a system of completeness checks to ensure that all relevant processes and events are represented and treated appropriately in the impact assessment
- uncertainty management that ensures relevant uncertainties are considered and either treated or their effects acknowledged
- easy accessibility to numerical simulators without prohibitive costs for acquiring it.

Regardless of the rigour in implementing model quality management processes, confidence in impact assessments can be no greater than the confidence in the scientific and technical understanding and information on which it is based.

An important path to achieving confidence in model simulations is to perform the numerical simulations in a way that is consistent with established principles and guidelines. As far as groundwater modelling is concerned, the Australian groundwater modelling guidelines (Barnett et al. 2012) provide a point of reference for groundwater flow and transport calculations. In the current exposure assessment the Australian groundwater modelling guidelines will be used as a guide for groundwater flow and transport calculations.

In addition, analysis and arguments providing complementary paths to confidence in model predictions include causal criteria analysis methods (Norris et al. 2008) and evidence from natural analogues (Chapman et al. 2000), especially if the long-term evolution of natural systems is of importance to the analysis.

6.1.1 Quality management, transparency and traceability

Quality management, including Quality Assurance and Quality Control (QA/QC) associated with numerical simulation are important because they provide the framework for producing modelling results that are traceable, reproducible, and defensible (Mallants et al. 2009; Perko et al. 2009b). QA generates confidence in a product by defining procedures under which work on the product is performed, and establishing a set of records that confirm that the procedures have been followed (ISO 2008). Furthermore, there is a need for a statement of the quality required of a product and its reproducibility.

Quality management, as applied to impact assessments, should also strive for *transparency*. Transparency means a report that should be written in such a way that its readers can gain a clear picture, to their satisfaction, of what has been done, what the results are, and why the results are as they are (NEA 1998). Impact assessments should also strive for *traceability*. Traceability requires an unambiguous and complete record of the decisions and assumptions made, and of the models and data (and its lineage) used in arriving at a given set of results (NEA 1998). Such properties help promote an efficient regulatory review and also build confidence in the results of the assessment. For an impact assessment to be sufficiently transparent and traceable for efficient regulatory review, the assumptions, uncertainties, rationale, and data used in it should all be readily available (NEA 1998).

Components of such quality management in regards to computer simulations include:

- software configuration
- data configuration
- application configuration.

Software configuration is intended to assure that:

- the code is sufficiently documented for external analysis
- the simulation software is performing satisfactorily with respect to the numerical implementation of governing equations

- the version of the code executable can be recovered such that the published results can be reproduced
- cost and origin of software should not be a factor determining accessibility to a simulator for the purpose of testing or reproducing model results.

Data configuration is intended to ensure that the selection of model input parameters is documented and traceable to maintained and / or referenced data sources, input data file versions are documented, maintained, and recoverable, and supporting software (e.g. geochemical calculations used to derive solubility limits) used to generate model parameters are documented, maintained, and recoverable (i.e. can be run at any time). Emphasis should be placed on the traceability of data to original sources and ensuring consistency between published data and code input parameter values relevant to the impact assessment.

Application configuration management is intended to:

- document and archive output files that are the basis for referenced results, tables, graphs, or figures intended for publication
- link simulation results to specific versions of the simulation software and input data files
- technically review simulations for the specific implementation of software and input data, as well as the veracity of the results.

In the current exposure assessment the reports will have a sufficient level of transparency and traceability allowing independent peer review. Proper QA procedures are in place that facilitate data provenance including linking reports to all underlying simulations results, cataloguing of such results and their archiving.

In addition, specific studies may be required to inform impact assessments, especially when higher tier assessments are invoked (see Figure 2.1). Examples of such studies for impact assessments dealing with leaching of contaminants from disposal ponds to groundwater include:

- site characterisation to determine hydrogeological and hydrogeochemical properties of the subsurface for which assessments are intended
- characterisation of chemical sources through monitoring of produced water from coal seam gas extraction
- sensitivity analyses, including supporting calculations, to provide better insight into relative importance of particular processes and parameters on chemical migration and their overall importance in the long-term fate of contaminants
- assessment of the behaviour of specific emerging contaminants in coal seam gas, such as degradation products
- reviews of the sorption mechanisms and sorption values for critical chemicals onto soil and sediment materials (Thibault et al. 1990; US EPA 1999).

In the current exposure assessment there is a sufficient level of scientific understanding of processes related to leakage of chemicals into the subsurface. A very thorough understanding of the scientific and technical basis for leaching of hydraulic fracturing fluids from surface impoundments and spills is available from several literature reviews carried out in the framework of this project (Mallants et al. 2017a; DoEE 2017a).

6.1.2 Qualification, verification and validation

6.1.2.1 Qualification and verification

Confidence in scientific and technical understanding is pivotal to obtaining confidence in impact assessments, but of equal importance is developing scientific confidence in the assessment models. This includes verifying whether the model is adequate, or ‘fit’, for its intended use; and whether or not there is sufficient evidence that the model development followed logical and scientific approaches. This includes ensuring it did not fail to account for important processes, future boundary conditions (such as climate), and operational conditions of remediation schemes, disposal operations, etc.

The key consideration in the selection of models, datasets (input parameters) and computer codes is that they should be *fit for purpose*. Judging fitness for purpose involves considerations of qualification, verification, and validation. The theoretical relation between these concepts is illustrated in Figure 6.1. Although not explicitly shown in Figure 6.1, the computer simulation step also involves model calibration: the process of adjusting numerical modelling parameters in the simulation model for the purpose of improving agreement with experimental data (AIAA 1998; Barnett et al 2012). Model calibration is generally followed by model validation using independent data (Refsgaard 1997; Xevi et al. 1997).

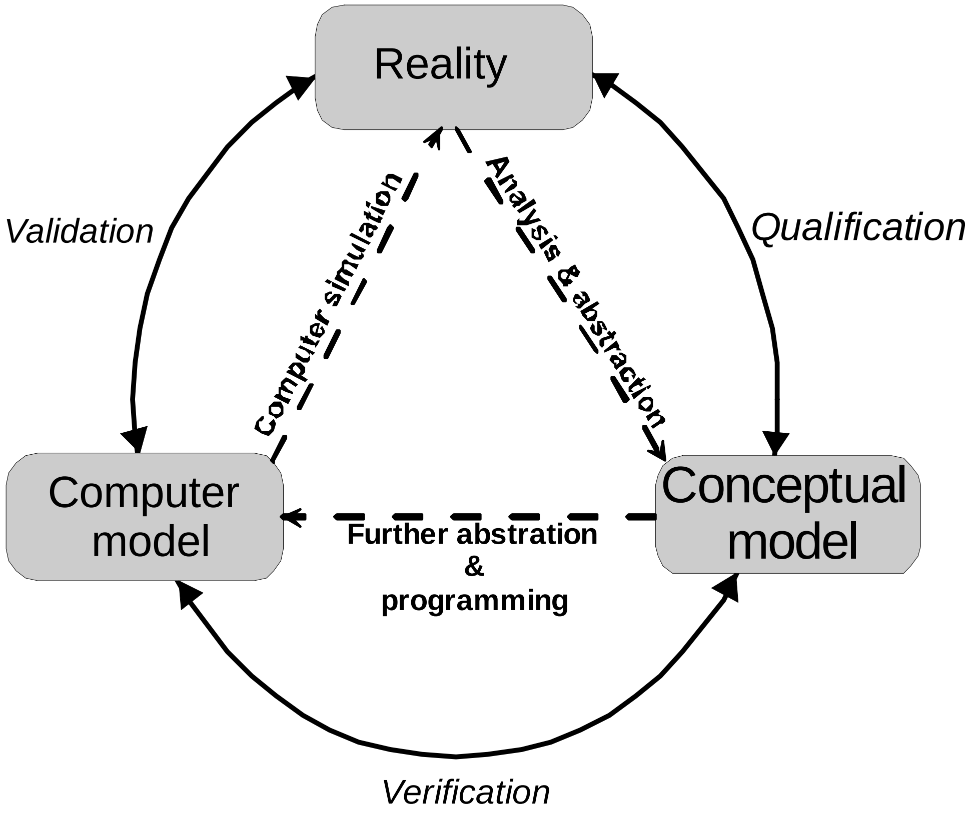
Qualification of a *conceptual model i*s defined as the process of ensuring that it is consistent with best available scientific understanding and adequately represents the phenomena and interactions relevant to its application or intended use (Sargent 2003).

The qualification of a *software code* is a mathematical issue with the goal of identifying and eliminating possible errors (such as programming errors). It is usually the code developer's responsibility to undertake this. It can be supported by general or specific software documentation (Sargent 2003).

General software documentation comprises supporting documentation such as users’ manuals or technical reference guides which also provide the theoretical basis and code structure. They should additionally describe modularity of models and flow of information between models which facilitates in-depth review as well as the domain and range of valid inputs.

Specific documentation includes peer reviewed journal papers which can enhance the validity of specific applications or model testing under alternative conditions. It is important to have evidence of this type, so as to provide confidence that assessment models will produce reasonable estimates of the future system responses.

Model verification is the process of determining whether a computer model correctly implements the intended conceptual model. In developing a computer model from a conceptual model, the simplifications made in deriving mathematical equations and boundary conditions must also be justified, which aids the goal of traceability. It must further be shown that the chosen computer code(s) solve the mathematical equations that define a case accurately and without error (Sargent 2003).



Modified after Sargent (2003)

Figure 6.1 Relationship between reality, conceptual model and computer model, and the concepts of qualification, verification and validation

Code verification, in this context, is the process of showing that the results generated by the code for simpler problems are consistent with the available analytical solutions, or are the same, or similar, as results generated by other codes (benchmarking) (Sargent 2003).

In the current exposure assessment the model qualification and verification are an integral part of the analysis and will be documented throughout the reports. Conceptual model qualification (testing if it adequately represents the phenomena and interactions relevant to its application) is currently foreseen for a realistic high end assessment commensurate with a Tier 1 analysis. The conceptual model was therefore simplified to ensure relevance to its application and intended use. Code qualification is based on existing general and specific documentation.

6.1.3 Validation

6.1.3.1 Definitions of validation

At present, there is no internationally agreed definition of model validation. In order to develop practical guidance on validation as part of a strategy for selecting and implementing simulation codes, it is useful to describe some of the existing approaches or views to validation. A summary of these definitions is given here, while a more detailed discussion is given in Appendix C:

- The scientific view of validation is that models are ‘true’ representations of reality. The most convincing evidence that a scientific theory or model is correct is through direct comparison of model predictions with experimental observations (US NRC 1984; US DOE 1986).

- The philosophical view refers to scientific legitimacy, rather than scientific 'truth'. In this sense, a valid model is one that does not contain known or detectable flaws and is internally consistent (Perko et al. 2009b).
- The regulatory view of model validation generally requires an adequate description of the phenomena for a given purpose. The adequacy of the model will then be a subjective decision to be made by the regulatory body (IAEA 2003a).
- The confidence building view defines the validation of impact assessment models as the process of building scientific confidence in the methods used to perform such assessment, recognising that this process requires many iterations between modellers and regulatory bodies (Perko et al. 2009b).

6.1.3.2 Validation strategy

Regardless of the differences in the views and definitions about validation, many focus on providing evidence that the model under consideration is adequate for its intended use. Furthermore, model validation is a long-term, iterative process aimed at building confidence in the model, which must rely on the processes of qualification and verification.

Very important in the validation process is the use of a diverse set of tests, designed to evaluate a diverse set of aspects related to the model. Validation tests should not be focused on whether the model is scientifically correct for all conditions, but rather on the adequacy of the model for the intended purpose.

The minimum requirement when validating assessment models is to establish an adequate scientific basis for regulatory credibility. Furthermore, the models should be sufficiently accurate for the purpose for which the model is used. This implies that each application of the model should be validated in a regulatory context. Because validation is a process rather than a single test, it is appropriate to develop a validation strategy to ensure a structured, transparent and traceable approach to validation. An important part of this is the project developer and the regulatory body reaching agreement on the degree of validation needed for each model used in the impact assessment and how best to achieve that degree of validation.

Overall, any model validation strategy should consider two aspects of model validation: a description of the activities implemented to gain confidence in those models used to demonstrate compliance; documentation of the results of those activities and the logic by which the conclusions were drawn (Wingefors et al. 1999; Perko et al. 2009b).

A key feature of a robust validation strategy is that the level of validation of a particular model or sub-model should be appropriate to the importance of that model or sub-model. The component most relied on to demonstrate compliance should be represented by a model with a higher degree of confidence and, thus, a higher degree of validation. Conversely, components less relied on will have models in which the confidence is less and therefore would need a lesser degree of validation. The decisions regarding the importance of models used should be transparent and documented.

In the current exposure assessment, model validation utilised the confidence building view and considered two distinct aspects: a description of the activities implemented to gain confidence in those models used to demonstrate compliance; and documentation of the results of those activities and the logic by which the conclusions were drawn. Central to this view was the need to demonstrate that the model is fit for purpose.

6.2 Uncertainty management

Uncertainty management is one of the cornerstones within an impact assessment. The management of uncertainties implies dealing systematically with uncertainties throughout the impact assessment and documentation of that process, and, thus, identifying priorities for additional work and topics for specific attention (NEA 1991).

By means of a systematic analysis of uncertainties, the following questions can be addressed:

- can the remaining uncertainties in the assessments jeopardise the health of humans or the environment?
- which uncertainties are being reduced in the different tiers of an assessment?
- which uncertainties can be reduced in the future?
- which uncertainties cannot or need not be reduced?

Some uncertainties simply cannot or need not be further reduced, but this does not necessarily hamper assessing their impact in a way that produces high end estimates. A typical example of the former is human behaviour in the far future, and long-term changes in hydrogeology and biosphere owing to human activities. Examples of the latter are those that have a negligible impact on chemical migration in groundwater, such as surface processes.

A systematic analysis of those uncertainties that potentially affect the impact of the system being investigated is done by treating uncertainties on three levels (Mallants et al. 2009):

- scenario uncertainties – are the (impact assessment) scenarios considered sufficiently complete in their representation of the possible evolution of the systems and its environment?
- model uncertainties – do the models describe the real world processes in an adequate way (in impact assessments we aim at not underestimating the impact)?
- parameter uncertainties – what impact do possible variations of the parameters have on the final results of the impact assessments?

For each of these three categories of uncertainty, the four questions discussed above should be addressed in the impact assessment. By means of sensitivity analysis and supporting calculations following a structured approach, the uncertainties that most affect the calculated response of the system or sub-system of interest can be identified. A sufficient collection of calculations should be carried out to ensure that there is confidence that the assessment has adequately covered the effects of combining assumptions relating to scenarios, models and input parameter values.

Guiding principles provided in the Australian groundwater modelling guidelines (Barnett et al. 2012) were adopted as much as was practical. Specifically, modelling results obtained in the National Assessment will be presented along with estimates of uncertainty, where feasible (Mallants et al. 2017b). While the Bioregional Assessments Program is developing procedures and workflows to manage uncertainties, these were not available at the time the National Coal Seam Gas Chemicals Assessment was carried out.

6.2.1 Treatment of uncertainty (scenarios, models, parameters)

While treating uncertainty aspects related to scenario development the following need to be addressed:

- completeness in terms of taking into account all possible relevant phenomena
- evolution in time
- uncertainties related to time frames and rates of disturbance processes.

This is addressed by developing and evaluating different scenarios, including the reference scenario and several scenarios with modified parameters. The reference scenario forms the basis for the development of all scenarios to be considered for impact assessments. For shallow groundwater a scenario with higher groundwater flow rates (high hydraulic conductivity and high hydraulic gradient) and minimal attenuation (no adsorption, degradation, etc.) would typically result in high end estimates. For deep groundwater a scenario with a hydraulically active fault that provides connectivity between coal seams and overlying aquifers would probably produce high end estimates.

Uncertainties on conceptual and numerical models are managed with specific procedures when selecting the models, datasets and computer codes in the impact assessments. Models should be fit for purpose. Selection of datasets (including input parameter values) is dependent on the mode of analysis, and whether deterministic or stochastic approaches are required. The most common approach has been deterministic assessments, whereby a so-called ‘best estimate value’, which represents the analyst’s or expert’s best judgement of what the (realistic) value of a given parameter should be under the conditions and assumptions of the scenario or assessment case, is selected. Then, in addition, a ‘high end estimate’ might be defined that represents a possible value, either higher or lower, but tending towards a value of the parameter that will have the effect of causing an overestimate of the impact, e.g. a shorter travel time from source to receiving environment, a higher solubility limit, or lower sorption coefficient.

In a probabilistic analysis, frequency distributions or probability density functions (PDFs), or ranges of input parameters, need to be defined. If the aim is to investigate sensitivity, then often uniform or log-uniform PDFs can be defined that span the possible range of a parameter value. If, however, an estimate of risk and uncertainty analysis is required, then greater attention needs to be given to defining the limits and form of the PDF to represent the best available knowledge of the key input parameters (those parameters that have been identified through judgement and the results of sensitivity analysis).

In the current exposure assessment the uncertainty in future system behaviour is addressed by applying high end scenarios. Uncertainty in parameter values is addressed by running multiple realisations (i.e. simulations). This accounts for realistic ranges of key chemical transport parameters for the flow and transport simulations in the unsaturated zone, and key hydrogeological parameters for the groundwater flow and solute transport calculations.

6.2.2 Evaluating conservatism

The inherent difficulty with evaluating conservatism (whether at the scenario, model, or parameter level) is that there is genuine uncertainty about what the real long-term behaviour, the real process, or real parameter value is. In many cases, a parameter for example might realistically take different values at different points in space or time. Therefore, assigning any single value is an approximation and the degree of approximation is not known because reality and its temporal and spatial evolution are not known. Similarly, the degree of overestimation induced by the choice of a high end input parameter is not known unless it can be established relative to some well-supported ‘realistic’ case.

Furthermore, it is important to recognise that the precise measurement of the degree of overestimation implies an absolute knowledge of reality and an ability to quantify how much we overestimate the consequences. Neither of these is possible in reality and so any measurement of the degree of overestimation must be seen as an approximate measure that has associated uncertainties. In other words: conservatism cannot be proven.

Therefore, it is important to document and justify the nature of each scenario, model, and data, and explain why it is considered high end or best estimate. Otherwise, if the nature of assumptions is not clearly documented, incorrect conclusions will be drawn from the assessment. This will further allow testing the likelihood that no unforeseen problems due to oversimplification will occur (e.g. processes not accounted for that may enhance mobility of contaminants such as changes in redox condition or complexing agents).

Despite these inherent difficulties in evaluating conservatism, where possible the nature of a high end assumption (whether on scenario, model, or parameter level) and its impact on system behaviour is indicated in the impact assessments. Although yardsticks for quantifying the level of overestimation introduced will usually not be readily available, attempts can be made to provide some reference condition to which the high end condition can be compared, and to compare modelled output with known upper bound incidents.

In the current exposure assessment the degree of overestimation due to model assumptions is demonstrated by comparing the simplified realistic, high end models to models that have a more complete description of processes relevant to chemical migration. This will be done for a limited number of cases (e.g. a leaching through soil scenario). This is different from benchmark calculations. Assessment results were also compared with reported incidents of spills and leaks (Mallants et al. 2017b).

6.2.3 Deterministic and stochastic calculations

There are two methods of quantitative analysis used in impact assessments: deterministic calculations and stochastic calculations (US NRC 1984).

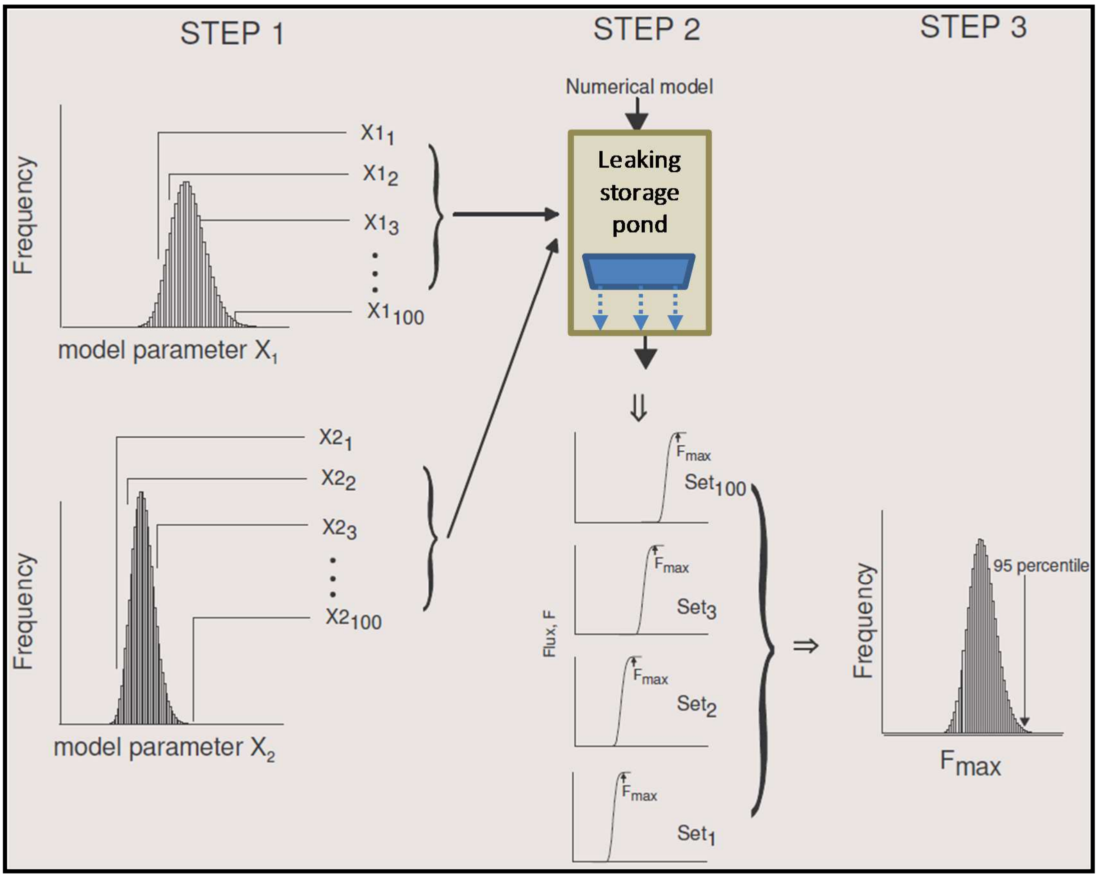
6.2.3.1 Deterministic calculations

A deterministic calculation employs a single value of each input parameter; this yields a single output value, time history or spatial distribution of the required output parameter. Deterministic analyses typically involve multiple deterministic calculations performed with the same model, each with a different input dataset, which yields multiple output values, time histories or spatial distributions, each for a specified and linked input dataset. This is typically done as a way of sensitivity analysis. Conclusions on the sensitivity of the output to individual input parameters, and the uncertainty generated by uncertainty in input parameter values, is achieved by comparison of the outputs.

6.2.3.2 Stochastic analyses

Stochastic analyses are done to evaluate parameter uncertainty, which typically includes both sensitivity and uncertainty analysis. In sensitivity analysis, the model input parameters are varied over sensible ranges to determine the effect of these variations on the result of the calculation. This increases our understanding of which parameters have to be determined with the greatest accuracy, and thus helps to prioritise data collection requirements. Sensitivity analysis provides a logical and verifiable method of optimising the distribution of resources used to determine the most important parameters. It also indicates which parameters have to be included in the uncertainty analysis.

Uncertainty analysis gives a numerical estimate of how the uncertainty in the input parameters results in uncertainty in the model results, i.e. uncertainty about fluxes, state variables, etc. (Figure 6.2). By means of an uncertainty analysis upper and lower confidence levels are obtained for specific model outputs, such as total flux at interfaces between environmental compartments, for a given set of uncertain model parameters.



Source: Mallants et al. (2009). The example shows the sampling of two parameters X_1 and X_2, the running of the soil transport model, and the statistical analysis of model output. Note that different types of distributions can be combined in the generation of parameter sets.

Figure 6.2 Illustration of Monte Carlo analysis

The example given in Figure 6.2 considers both sensitivity and an uncertainty analysis, based on a stochastic modelling approach. For this purpose a sufficiently large sample is drawn from the theoretical parameter probability density functions. One powerful parameter generation technique is the Latin Hypercube Sampling (LHS) method. The LHS uses a stratified way of sampling from separate sampling distributions on the basis of a subdivision in intervals of equal probability, resulting in an efficient, and therefore, relatively small number of samples.

Figure 6.2 used an LHS size of 100 to ascertain a perfectly representative sample (i.e. ‘observed’ statistical parameters agree with theoretical PDF parameters). With these 100 sets of parameter values 100 runs with the numerical flow and transport model are made and the 100 model outputs are analysed statistically in terms of the partial rank correlation coefficient (PRCC) and percentile values (e.g. 95^{th}, 50^{th} percentile). This whole analysis is also referred to as Monte Carlo (MC) analysis.

In the sensitivity analysis illustrated in Figure 6.2, results from the Monte Carlo analysis (i.e. the entire set of model outputs) are used to calculate statistical estimators of the sensitivity between model parameters and model outputs, for example between flux from a disposal pond to groundwater and the soil-water partition or distribution coefficient K_d. One powerful estimator is the partial rank correlation coefficient (PRCC; for details, see Hamby 1995). The meaning of the PRCC is explained by considering the following: if a large number of runs are made with parameter values changing simultaneously, it is difficult to assess the sensitivity of the model output Y to the individual variable Xj. The partial correlation coefficient provides the means to quantify this sensitivity. The difference between a simple correlation coefficient and the partial correlation coefficient is that the latter measures the degree of linear relationship between X_j and Y thereby removing the linear effect of all other remaining parameters. In other words, from the partial correlation coefficient one can obtain the unique contribution of one particular parameter. To avoid problems of nonlinearity between X_j and Y and problems due to values covering a range of several orders of magnitude (possibly due to outliers), the original variables are replaced by their corresponding ranks. The partial correlation coefficient calculated on these ranks is the partial rank correlation coefficient. This parameter allows obtaining a ranking of the parameters' importance in affecting the system investigated (e.g. Seuntjens et al. 2002).

In the current exposure assessment, deterministic calculations were developed while stochastic calculations were approximated by running multiple simulations accounting for a limited number of parameter perturbations. The latter approach is referred to as factorial design. The factorial design technique is another way to deal with parameter uncertainty (Saltelli et al. 1993). This computationally less demanding technique allows a quick screening of parameter combinations, from which the most sensitive ones can be obtained. If one chooses a factorial design with two parameters and three levels (i.e., minimum, best estimate or reference, and maximum value), then the number of parameter combinations and model runs is defined as $3^2 = 9$. For three parameters and three levels the number of models runs is $3^3 = 27$. This approach will be used to determine the effect of parameter uncertainty on migration in the subsurface (soil and shallow groundwater models).

7 Conclusions

Exposure assessment of chemicals leaking from surface sources into soil and shallow groundwater requires contaminant pathway modelling from the chemical source (such as low-rate leakage from surface ponds containing flowback and produced water) to different receiving environments (such as water wells, rivers, and wetlands) across the landscape. Prior to developing numerical models of solute or chemical transport, conceptual models needed to be developed that reflect current understanding of a complex soil-groundwater system for an intended purpose. Conceptual models for water flow and solute transport through the unsaturated zone and groundwater are presented, including a description of the domain geometry, initial and boundary conditions, model parameters as well as auxiliary information to put the simulation results (that is predicted environmental concentrations) in a likelihood context.

The Namoi sub-bioregion was selected as case study area for the purpose of demonstrating the exposure assessment framework associated with leakage of hydraulic fracturing fluids from surface sources. The area has several key relevant receiving environments in a relatively small area facilitating the use of a limited number of models to represent a broad range of receiving environments. Furthermore, coal seam gas extraction is being trialled and is expected to be developed across a relatively large area which includes important receiving environments for humans and the environment. Finally, existing groundwater flow models could be relatively easily adapted and made fit for purpose within the short timeframe of this project.

The unsaturated zone in the alluvial planes is mainly made up of heavy textured soils with a depth to groundwater table between approximately 1 and 30 m in the selected case study areas. Different thicknesses of the unsaturated zone will be considered in the exposure assessments to account for the observed variability in depth from the land surface to the groundwatertable. The conceptual model allows calculation of a solute concentration and the subsequent derivation of a dilution factor at any point in the unsaturated zone, including at the interface with the groundwatertable.

The conceptual model for the unsaturated zone has provisions to account for different solute sources at the land surface and their characteristics previously identified. Solute transport across the unsaturated zone was conceptualised by applying the advection-dispersion equation for an imposed water flux equal to the assumed leak rate followed by an average groundwater recharge rate representative of soil conditions after dismantling of the storage ponds. Based on an extensive literature survey, three leak rates for single-lined ponds under normal operations were identified for subsequent exposure assessments: 0.35, 3.5 and 35 mm/year (Rowe and Hosney 2010; Rowe 2012). The 0.35 mm/y leak rate could be considered a reference value for liner designs that include a composite geomembrane / geosynthetic clay liner. The 3.5 mm/y leak rate on the other hand is more representative for a composite geomembrane / compacted clay liner. Finally, the 35 mm/y leak rate is typical for a design with a single geomembrane liner or a compacted clay liner with a similar hydraulic conductivity. Current pond and liner designs from some coal seam gas companies were consulted and compared to the classification developed from the literature survey (AE 2008; Clarke 2008; RPS 2012). This allowed assigning (very low) leak rates to the various designs commensurate with data from international studies (Beck 2012a, b).

A three-dimensional numerical groundwater flow model previously developed during the Namoi Catchment Water Study was used as the basis for developing a conceptual model for chemical assessment. As the Namoi Catchment Water Study is relatively recent, well documented, and has a rigorously tested alluvial aquifer model component with very good model performance, it was selected as the one to be adapted and used for the purposes of calculating environmental concentrations of hydraulic fracturing and drilling fluids associated with spills and leaks. The regions of the catchment underlain by the alluvial aquifers are relevant for exposure assessment of chemicals leaking from the soil surface into shallow groundwater. Furthermore, in these regions the model can be relatively easily adapted to fit the requirements for solute transport simulations, that is the numerical grid has to be sufficiently small i) to reduce numerical dispersion and oscillations, ii) to allow proper representation of large concentration differences over short distances, and iii) to allow proper representation of solute sources and receiving environments.

For the purpose of determining solute transport in groundwater in the exposure assessments, two local groundwater flow models were “cut out” of the regional Namoi Catchment Groundwater Model. Within one of these local models, an even smaller site model will be developed as part of the exposure assessments with a refined numerical grid to allow accurate calculation of solute migration. Selection of the preferred local model was based on the following criteria: i) potential risk to humans and the environment based on ongoing and planned activities in regards to coal seam gas extraction, ii) the area has to be sufficiently representative in terms of broad coverage of hydrogeological features, and iii) the area has to be sufficiently representative in terms of receiving environments of relevance to both human and environmental receptors. Based on these criteria, an area of 45 km by 67 km, including the Namoi river, has been selected for further exposure assessments. It contains shallow groundwater and shallow water wells in the alluvial aquifer, groundwater dependent wetlands, and a gaining river section.

As a starting point for the groundwater flow simulations, the calibrated Namoi Catchment Groundwater Model will be used to develop the two local models. Spatial variation in key flow and transport parameters from these two local models will be analysed to inform relevant parameter variations that will be used to generate multiple parameter sets. Such parameters will then be used to generate multiple flow and transport simulations of the refined site model. These simulations will determine the likely range of predicted environmental concentrations or derived dilution factors for key receiving environments typical of shallow groundwater systems. The results can be extrapolated to a larger area than the domain used in the calculations, provided i) the larger area hydrogeological conditions can be quantified in broad classes of groundwater velocity and travel times from source to receiving environment, and ii) a sufficient similarity exists in groundwater velocity and travel times between the simulation domain and the larger areas.

To assess the likelihood that a particular receptor (i.e. a water well, an endangered plant or an endangered animal species) would be within a given distance from a coal seam gas well (the location of the coal seam gas well is assumed to be the location of the contaminant source), a spatial analysis was undertaken considering radial distances between coal seam gas wells and receptors from 100 to 10 000 m. This allows determination, for the currently known locations of coal seam gas wells and receptors in the Namoi catchment, of the likelihood of a receptor being within a potential contamination plume.

For water wells, the cumulative empirical distribution function reveals there is only a 1% chance of finding water wells within a distance of approximately 600 m of a coal seam gas well, or conversely, in 99% of all cases wells will be at distances greater than approximately 600 m from a coal seam gas well. The closest distance reported between a coal seam gas and a water well is 100 m. The probability of this occurring is only 0.03% (10 out of a total of 34 215 wells with a screen depth less than 50 m).

For endangered flora species, the cumulative empirical distribution reveals there is only a 1% chance of finding such species within a distance of approximately 350 m of a coal seam gas well, or conversely, in 99% of all cases endangered flora species will be at distances greater than approximately 350 m from a coal seam gas well. The closest distance reported between a coal seam gas well and an endangered flora species is 200 m. The probability that this occurs is only 0.4%.

For water dependent animal species, the cumulative empirical distribution reveals there is a 1% chance of finding such species within a distance of approximately 180 m of a coal seam gas well, or conversely, in 99% of all cases water dependent animal species will be at distances greater than approximately 180 m from a coal seam gas well. The closest distance reported between a coal seam gas well and a water dependent animal species is 100 m. The probability that this occurs is 0.4%.

A comprehensive framework to build confidence in numerical modelling and its reporting has also been presented. Elements of confidence building in quantitative impact assessments include:

- rigorous record keeping and quality assurance procedures to ensure the calculations and results are those intended, and are fully traceable and reproducible
- scientific and technical understanding of the processes and events involved, i.e. justification of the information that is compiled in the assessment basis
- models, codes and data that are ensured through the verification, qualification and, when possible, validation process
- a system of completeness checks to ensure that all relevant processes and events are represented and treated appropriately in the impact assessment
- uncertainty management that ensures relevant uncertainties are considered and either treated or their effects acknowledged
- easy accessibility to numerical simulators without prohibitive costs for acquiring it.

Uncertainties associated with the soil and groundwater flow and transport models mainly relate to uncertainties about model parameters used and uncertainties about the conceptual model that was initially developed. A first step to address uncertainties associated with the model parameters was undertaken by identifying a range of plausible parameter values based on the Namoi Catchment Groundwater Model. When exposure calculations are undertaken, soil and groundwater models will be run multiple times using those different parameter values to quantify propagation of parameter uncertainty through a model to affect the model output uncertainty. Uncertainties in the conceptual model were addressed by developing simplified conceptual models based on high end estimates of parameters that are not likely to underestimate impact. Accounting for the effects of uncertainty analyses will also help to bracket the range of solute concentrations that key receptors may be exposed to.

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Appendix A – Namoi Catchment Model Hydraulic parameters

Table A 1 Final values used in the Namoi Catchment Model from Schlumberger Pty Ltd. Layer type: U = unconfined, C = confined.

Layer #	Geological equivalent	Layer type	Horizontal conductivity (m/day) min–max (average)	Vertical conductivity (m/day) min–max (average)	Specific yield min–max (average)	Specific storage (m^{-1}) min–max (average)
1	Narrabri	U	0.001-30 (4.72)	0.00005-0.5 (0.177)	0.005-0.25 (0.059)	0.000001-1 (0.536)
2	Gunnedah	U	0.001-0.1 (0.062)	0.00001-0.001 (0.0001)	0.01-0.1 (0.07)	0.000001-0.00001 (0.0000073)
3	Lower Namoi Alluvium/ weathered horizon	U	0.001-0.1 (0.062)	0.00001-0.01 (0.000951)	0.01-0.1 (0.07)	0.000001-0.00001 (0.0000073)
4	Fractured rock horizon	U	0.001-0.1 (0.054)	0.00001-0.001 (0.00015)	0.01-0.1 (0.02)	0.000001-0.000005 (0.0000046)
5	Great Artesian Basin	U	0.001-0.05 (0.037)	0.00001-0.001 (0.00015)	0.01-0.1 (0.03)	0.000001-0.000005 (0.0000046)
6	Pilliga sandstone	U	0.001-0.02 (0.01)	0.00001-0.001 (0.00015)	0.01-0.1 (0.08)	0.000001 - 0.000005 (0.0000046)
7	Purlawaugh	U	0.001-0.02 (0.011)	0.00001-0.001 (0.00022)	0.01-0.1 (0.08)	0.000001-0.000005 (0.0000046)
8	Garrawilla volcanics	U	0.001-0.02 (0.017)	0.00001-0.001 (0.00084)	0.01-0.1 (0.07)	0.000001-0.000005 (0.0000046)
9	Napperby and Deriah	U	0.001-0.02 (0.016)	0.00001-0.001 (0.00078)	0.01-0.15 (0.1)	0.000001-0.000005 (0.000004)
10	Digby	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00016)	0.01-0.1 (0.07)	0.000001-0.000005 (0.0000043)
11	Upper Black Jack	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00016)	0.01-0.15 (0.1)	0.000001-0.000005 (0.000004)
12	Hoskinssons seam	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00016)	0.01-0.1 (0.07)	0.000001-0.000005 (0.0000013)
13	Middle Black	U	0.001-0.01	0.00001-0.001	0.01-0.15	0.000001-0.000

Layer #	Geological equivalent	Layer type	Horizontal conductivity (m/day) min–max (average)	Vertical conductivity (m/day) min–max (average)	Specific yield min–max (average)	Specific storage (m^{-1}) min–max (average)
	Jack		(0.0085)	(0.00016)	(0.1)	005 (0.000004)
14	Melvilles seam	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00016)	0.01-0.025 (0.016)	0.000001-0.000 005 (0.0000013)
15	Lower Black Jack	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.0008)	0.01-0.025 (0.016)	0.000001-0.000 005 (0.0000035)
16	Watermark and Porcupine	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00048)	0.01-0.025 (0.016)	0.000001-0.000 005 (0.0000026)
17	Maules Creek Upper Buffer	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00048)	0.01-0.025 (0.016)	0.000001-0.000 005 (0.0000026)
18	Maules Creek	U	0.001-0.01 (0.0085)	0.00001-0.001 (0.00048)	0.01-0.025 (0.016)	0.000001-0.000 005 (0.0000026)
19	Maules Creek Lower Buffer	C	0.001-0.01 (0.0082)	0.00001-0.001 (0.00082)	0.01	0.000001-0.000 005 (0.0000026)
20	Leard	C	0.001-0.1 (0.062)	0.00001-0.001 (0.0001)	0.01-0.1 (0.07)	0.000001

Appendix B – Groundwater dependent ecosystem data

Vegetation that rely on subsurface presence of groundwater from the National Atlas of Groundwater Dependent Ecosystems (2013). Data relevant for Namoi catchment:

- Acacia
- Alectryon/Rusty Fig/Mock Olive Dry Rainforest; scattered
- *Allocasuarina leuhmannii* (Bull Oak)
- Alpine Gum
- Angophora floribunda
- Apple-Black Cypress
- Apple-Manna Gum woodland
- Barrington Wet New England Blackbutt-Blue Gum
- Belah/White Pine Shrubby Woodland (with patches of Semi-evergreen Vine Thicket); north-west
- Bimble Box/White Pine Grassy Woodland; western
- Black Pine - Narrowleaf Ironbark - Bloodwood - Red Gum (blakeyi) (Western Region)
- Black Pine Granite Outcrop Shrubby Woodland; tableland edge
- Black Pine/Orange Gum/Tumbledown Red Gum Shrubby Open Forest; south-east
- Black Pine/Tumbledown Red Gum/Caley's Ironbark Shrub/Grass Open Forest; widespread
- Black Pine/White Box Shrubby Open Forest; Kaputar
- Blakely's Red Gum/Rough-barked Apple/Red Stringybark Grassy Open Forest; tableland edge
- Blakely's Red Gum/Yellow Box Grassy Open Forest/Woodland; tablelands
- Blakely’s Red Gum (+ Rough-barked Apple)
- Bloodwood - Broadleaf Ironbark - White Cypress Pine - (Black Pine) (Western Region)
- Box dominated forest and woodland
- Broad-leaved Stringybark
- Brown Barrell-Gum
- Brown Bloodwood/Broadleaved Ironbark/Cypress Pine spp.
- Bull Oak
- *Callitris glaucophylla*
- *Casuarina cunninghamiana*
- Central Mid Elevation Sydney Blue Gum

- Cool Moist Messmate
- Corkwood-Crabapple and Mixed Stringybarks
- Corymbia trachyphloia
- Cypress Pine
- Diehard Stringybark-New England Blackbutt
- Dry Grassy Stringybark
- Dry Open New England Blackbutt
- Dry Rainforest types
- Dry Redgum-Bloodwood-Apple
- Dry Silvertop Stringybark-Apple
- *E.albens* grassy woodland
- *E.macrorhyncha* grassy forest/woodland
- *E.microcarpa* and / or *E.pilliga*
- Escarpment Redgum
- Escarpment Scribbly Gum-Apple
- *Eucalyptus albens*
- *Eucalyptus blakelyi*
- *Eucalyptus camaldulensis*
- *Eucalyptus coolabah*
- *Eucalyptus crebra*
- *Eucalyptus dealbata* and / or *Eucalyptus dwyeri*
- *Eucalyptus fibrosa*
- *Eucalyptus laevopinea*
- *Eucalyptus largiflorens*
- *Eucalyptus melanophloia*
- *Eucalyptus melliodora*
- *Eucalyptus microcarpa*
- *Eucalyptus nortonii*
- *Eucalyptus pauciflora*
- *Eucalyptus pilligaensis*
- *Eucalyptus populnea*
- *Eucalyptus spp*
- *Eucalyptus trachyphloia*
- Gorge Grey Box
- Gramminoid complex

- Granite Mallee
- Grassy New England Blackbutt-Tallowwood-Blue Gum
- Grassy White Box types
- Grey Box/Blakely's Red Gum/Yellow Box Grassy Open Forest; widespread
- Grey Gum-Stringybark
- High Elevation Messmate-Brown Barrell
- High Elevation Moist Open Tallowwood-Blue Gum
- Hill Red Gum types
- Ironbark dominant forest and woodland
- Kurrajong/Not present/Not present
- Mallee-Peppermint
- Manna Gum
- Messmate
- Messmate-Mountain Gum Forest
- Mid North Coast Wet Brushbox-Tallowwood-Blue Gum
- Mixed Tableland Stringybark-Gum Open Forest
- Moist Escarpment New England Blackbutt
- Moist Open Escarpment White Mahogany
- Montane Stringybark-Gum
- Mountain/Manna Gum
- *Muehlenbeckia florulenta*
- Mugga Ironbark/Blakely's Red Gum Shrub/Grass Open Forest; Bingara
- Myrtle Shrubland (+- White Pine/Tumbledown Red Gum); Dripping Rock
- Nandewar Box/New England Blackbutt/Red Stringybark Shrub/Grass Open Forest; Kaputar
- Narrow-leaved Ironbark/Brown Bloodwood/Red Stringybark
- New England Blackbutt forest types
- New England Stringybark-Blakelys Red Gum
- Open Ribbon Gum
- Open Silvertop Stringybark-Blue Gum
- Open Tumbledown Gum-Black Cypress-Orange Gum
- Orange Gum-Ironbark
- Outcrop Orange Gum-New England Blackbutt
- Paperbark Riparian Forb/Grass Low Closed Forest; widespread
- Peppermint

- Rainforest
- Red Gum-Apple
- River Oak Riparian Open Forest; widespread
- River Red Gum Riparian Open Forest/Woodland; widespread
- Rock outcrop vegetation
- Rough-barked Apple dominant
- Rusty Fig Dry Rainforest; scattered
- Scattered trees
- Semi-evergreen Vine Thicket; scattered
- Shrubby White Box types
- Silverleaf Ironbark - White Cypress Pine (Lindsay Types)
- Silvertop Stringybark/Bendemeer White Gum Grassy Open Forest; Kaputar and southern tableland edge
- Silvertop Stringybark/Orange Gum Shrubby Open Forest; Horton
- Silvertop Stringybark/Rough-barked Apple Grassy Open Forest; southern hills
- Snow Gum
- Stringybark-Apple
- Swamp
- Tableland Gums/Peppermints
- Tumbledown Gum/Black Pine/Acacia cheelii Shrubby Open Forest; scattered
- Weeping Myall Woodland/Shrubland; scattered
- White Box
- White Cypress Pine
- White Pine/Narrow-leaved Ironbark Shrub/Grass Open Forest; south-west
- Yellow Box-Blakely's Red Gum

Appendix C – Validation

Approaches to validation

Scientific view

The scientific view of validation usually means that models are 'true' representations of reality. The most convincing evidence that a scientific theory or model is indeed correct is through direct comparison of model predictions with experimental observations. Broadly two approaches to model validation have been developed among the scientific community:

- a pragmatic, *positivist* approach in which acceptance of a scientific theory depends more on achieving consensus (after Kuhn 1970), and
- a restrictive, *negativist* approach which implies that a theory cannot be verified, only falsified (after Popper 1968).

Proponents to the first approach, such as Neuman (1992) argue that positive evidence also contributes significantly to validation of models, where 'positive evidence' means that a model has met with repeated success in explaining pertinent observations and experimental data. Furthermore, the process of model validation is:

> *"the gradual building of confidence among scientists, and thereby among the public, that understanding is being developed on the basis of a research program".*
>
> *Source: Neuman (1992)*

The best way to achieve consensus that confidence is warranted is through a careful validation of all models that are used in isolation, regardless of how complex or simplified their components are. To put it simply: a scientific theory by definition is true if it has gained broad consensus among the experts of that particular science.

A typical example is the variably saturated flow and transport code HYDRUS (Šimunek et al. 2006, 2008), which has been shown with satisfaction to explain laboratory and field data for a wide range of contaminants, in various physical-chemical environments and under a variety of initial and boundary conditions.

Proponents of the second approach include Davis et al. (1991), stating that the model will retain the status of being 'not invalid' until experimental evidence is obtained that clearly rejects the validity of the model. Or, in other words, showing that a model is not incorrect builds confidence that the model is an adequate representation of the real system and acknowledges that perfection is not possible.

Philosophical view

According to the philosophical view of model validation, the term does not refer to establishment of (scientific) truth but rather legitimacy. In this sense, a valid model is one that does not contain known or detectable flaws and is internally consistent.

By using as numerous and diverse confirming observations as possible, it is not unreasonable to conclude that at least the concept is not flawed. In other words, by using as much data as possible, attempts must be made to invalidate a model demonstrating it is either certain or uncertain beyond reasonable doubt.

Regulatory view

Tsang (1991) argues that it is illogical to refer to a validated model in the generic sense, but it can be stated that a model is validated with respect to a given process, or a group of models are validated with respect to a given site.

According to Zuidema (1994) it is not critical that models are strictly correct and include all natural details and processes, but that any uncertainty and simplification results in overestimating the consequences (concept of producing high end estimates). Further, an approach which overestimates the consequences is not a static idea: high end assumptions (imposed because of lack of data or insufficient understanding of processes and future drivers) can be replaced by more realistic ones when more information becomes available.

The concept of deliberately overestimating consequences and the requirement that models need to go through a validation process, represent two processes aiming at assuring the public that decisions made based on model results lessen the risk of compromising public health and safety.

Therefore, in the context of exposure assessments, regulatory bodies often require ‘reasonable assurance’ that the models comply with regulatory criteria. This concept recognises that absolute assurance of compliance is neither possible nor required, but model developers should provide all information necessary to convince a ‘reasonable decision maker’ that compliance with regulatory criteria would be achieved. For example, in the case of a site-specific assessment, no (or low) confidence will be expressed in a model that is used to extrapolate beyond the envelope of the values in the dataset used to establish the calibrated version of the model.

Thus, the regulatory expectations for model validation generally require only an adequate description of the phenomena for a given purpose. The adequacy of the model will then be a subjective decision to be made by the regulatory body.

Confidence building view

Validation of impact assessment models can be defined as the process of building scientific confidence in the methods used to perform such assessment, and recognises that this process requires many iterations between modellers and regulatory bodies. The main concerns should always be:

- whether or not the model is adequate for its intended use
- whether or not there is sufficient evidence that the model development followed logical and scientific approaches and did not fail to account for important processes.

Operational definitions of validation

Given the disagreement on the definition of validation, several organisations have developed *operational definitions* of validation. For example, the U.S. Nuclear Regulatory Commission has defined validation as:

> *“the process of obtaining assurance that a model, as embodied in a computer code, is a correct representation of the process or system for which it is intended”.*
>
> *Source: US NRC (1984)*

The Swedish Nuclear Power Inspectorate (SKI) has used the definition:

> *"validation is the testing of a model in a real world",*
>
> *Source: Nicholson (1990)*

which is also close to the definition put forward by the U.S. Department of Energy:

> *"validation of computer codes and models is a process whose objective is to ascertain that the code or model indeed reflects the behaviour of the real world."*
>
> *Source: US DOE (1986)*

The definition given by the IAEA in the context of radioactive waste management (IAEA 2003a) focuses on adequacy or 'fitness for purpose', that is validation is the process of building confidence that a model adequately represents a real system for a specific purpose. Hereby, it is understood, that model predictions are compared to observations or measurements on relevant systems, so model parameter uncertainty can be reduced. It is acknowledged, however, that the validation of models for the long-term evolution of a specific site is not possible over such long time scales (IAEA 2008a).