Risk Assessment Methodology for Underground Coal Gasification Technology

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Abstract

Geoenergy technologies, including the Underground Coal Gasification (UCG), are currently being considered as possible solutions for reducing emissions of CO_2 and other gases to atmosphere and at the same time, provide sustainable sources of low-carbon energy. In this paper, a flexible risk assessment methodology for UCG technology is presented, based on an established methodology for radioactive waste repositories. The assessment methodology can be applied at any stage in a project, between initial planning and final site abandonment. Central to the approach is the analysis of scenarios, which represents a “source-pathway-receptor” combination and its evolution. Here, a Reference Scenario (RS) and several Alternative Scenarios (AS) are developed and analysed using a numerical model. Results of the RS suggest that contaminant concentrations at an evaluation point are far below any level that could reasonably be detected. In some AS, the calculated concentrations showed an increasing trend at the end of the assessment period, potentially approaching levels that conceivably could be detected. However, as such cases are unexpected and pessimistic, their inclusion is to illustrate worst cases that could happen, rather than to give predictions. An illustrative application demonstrates that plausibly the risks of groundwater contamination from a UCG site should be very low if the site is developed and operated appropriately. The outcomes from applying the numerical model are intended to demonstrate how the methodology and the numerical model can be readily adapted to different sites.

Keywords: Geoenergy, Risk Assessment, Underground Coal Gasification, Environmental impact, Numerical Modeling, Groundwater contamination

1 Introduction

A rising number of countries and companies are targeting net-zero greenhouse gas emissions by 2050 in order to minimise global warming and avoid its worst environmental effects. The International Energy Agency (IEA, 2020) suggest that if today's energy infrastructure continues to operate as it has in the past, it would lock in by itself a global atmospheric temperature rise of 1.65°C. To prevent that, the decarbonisation of electricity production, transport, heating, and industry to meet the international climate change targets is a major challenge the world is currently facing. However, for many reasons it is not practical in all parts of the world to deploy zero-carbon technologies immediately and a portfolio of transitional low-carbon technologies will be needed to reduce greenhouse gas emissions as rapidly as possible.

According to the International Energy Agency (IEA, 2018; 2020), there is a pressing need to accelerate the development of low-carbon energy technologies to address this challenge. Geoenergy encompasses novel energy technologies and geological sources, such as Carbon Capture and Storage (CCS); radioactive waste disposal; air, heat and hydrogen storage; geothermal heat; and conventional and unconventional hydrocarbons. For instance, Underground Coal Gasification (UCG), a method for unconventional exploitation of fossil fuels, has been recognised as one of the technologies that can enable production of high calorific gaseous products in a sustainable manner (Bhutto et al., 2013). Nevertheless, these technologies require understanding of the geological and engineering controls and risks related to injection, extraction or interaction with fluids, for their responsible and safe utilisation to achieve a low-carbon future.

For a number of these geoenergy technologies, a lot of work has been done to assess and understand the risks associated with their usage, and as a result, such technologies are being commercialised or are on a path to commercialisation (Maul et al., 2007; Metcalfe et al., 2008; Little et al., 2009; Paulley et al., 2011; Tucker et al., 2013; Farr et al., 2016; Brabham et al., 2020; Heinemann et al., 2021; Zweigel et al., 2021). However, the UCG technology, which has been tested and piloted worldwide for more than 60 years (e.g. Perkins, 2018), is yet to be commercialised. UCG has been identified as a technology that can provide gas for electricity generation and for use as a chemical feedstock, and a source of hydrogen and methane for producing "blue" hydrogen (Stańczyk et al., 2012; Sarhosis et al., 2017; Kapusta et al., 2020; Sadasivam et al., 2020a). In addition, an attractive solution is to combine UCG with CCS so that CO_2 generated from UCG-related processes is reinjected back underground in the UCG cavities, adjacent unmineable coal seams and destressed geological formations (Younger, 2011; Man et al., 2014; Yang et al., 2016).

UCG is commonly deemed to be a clean coal technology (Attwood et al., 2003; Xie et al., 2020). However, it is essential to deploy UCG in such a way that it poses no risk to groundwater. Groundwater contamination is considered to be the most serious plausible negative environmental impact of UCG, which can produce and release organic contaminants such as phenol, benzene, toluene, ethyl benzene, xylene (BTEX) and polycyclic aromatic hydrocarbons (PAH) along with inorganic metals, metalloids, non-metal and anionic compounds (Kapusta and Stańczyk, 2011; Smolinski et al., 2012; Imran et al., 2014; Kapusta et al., 2015; Sadasivam et al., 2020b; Ma et al., 2021). The change of groundwater quality, particularly during the decommissioning and post-abandonment stages, has been observed in a number of field investigations, such as Hoe Creek trial (Campbell et al., 1978; Dalton and Campbell, 1978), Hanna site (Lindblom and Smith, 1993), and Barbara coal mine (Kapusta et al., 2013). Most recently, the Queensland Government inherited responsibility for the management of a UCG site in Hopeland after the operator caused environmental harm and failed to comply with the Environmental Protection Act 1994 (Queensland Government, 2021).

To understand the environmental impact of UCG, An et al. (2021a,b) and Zagorščak et al. (2019) conducted a preliminary risk assessment of UCG in deep-buried seams, however the assessment timeframe was limited to the gasification phase and 10 years after the gasification termination. Similarly, Soukup et al. (2015) and Šolcová et al. (2009) studied contaminant transport in porous media in the vicinity of the UCG reactor using assessment timeframes of up to 50 years. Beath et al. (2004) evaluated some geotechnical and hydrological impacts of UCG at the near-field and regional scales, using assessment timeframes of up to 1,000 years. However, the abovementioned studies did not consider the long-term evolution of UCG, including any features (system components), events and processes that might affect such evolution.

Generally, a regulator will require the potential for contamination to be assessed at some specified location and the assessment methodology should consider a sufficiently long time that peak risks, and the time at which they occur, can be estimated. Developing a structured and transparent assessment methodology to understand the long-term environmental impact of UCG can help to achieve that. The results of the risk assessment conducted by using such methodology could help to inform a range of stakeholders such as national and local governments, regulatory authorities, scientific bodies, and members of the public.

The risk assessment presented here is based on an established methodology for radioactive waste repositories (IAEA, 2004) and can be applied at any stage in a project. The overall approach is based on a source-pathway-receptor analysis. For illustrative purposes, the methodology assumes that a European regulatory regime will apply. However, the methodology can be readily applied under other regulatory regimes elsewhere in the world.

2 Methodology

2.1 Assessment Context

The principal purpose of the assessment methodology presented in this work is to assess the levels of environmental risk associated with UCG, primarily in the long-term, following abandonment of a UCG site. However, the development and operational phases of a UCG project need to be considered in so far as activities undertaken in these phases could impact upon long-term risks post-abandonment. In risk assessments of other waste generating technologies, such as radioactive waste disposal, the assessment methodology needs to consider a sufficiently long time that peak risks, and the time at which they occur, can be estimated. Here, 10,000 years have been considered, although the methodology can be extended readily to longer timescales if required by regulators or other stakeholders. The main stages of the assessment methodology are outlined in Figure 1 (IAEA, 2004). The methodology for the risk assessment presented here is based on international best practice, as embodied in the standards and recommendations of the International Atomic Energy Agency (IAEA, 2004). The approach undertaken enables comparison of results with potential regulatory requirements, enables uncertainties to be identified and analysed, and provides a framework for further amendments and review.

The assessment philosophy is to determine pessimistic (conservative) values of the agreed risk metrics for both a reference (or expected) system evolution and unexpected, but plausible, alternative system evolutions. A source-pathway-receptor analysis approach is used, whereby the underground region of coal gasification is a potential source of pollutants. All plausible pathways for pollutant migration from this source to potential receptors are then analysed. The receptors for the purpose of the assessment are surface water bodies and groundwater outside the immediate vicinity of the coal gasifier.

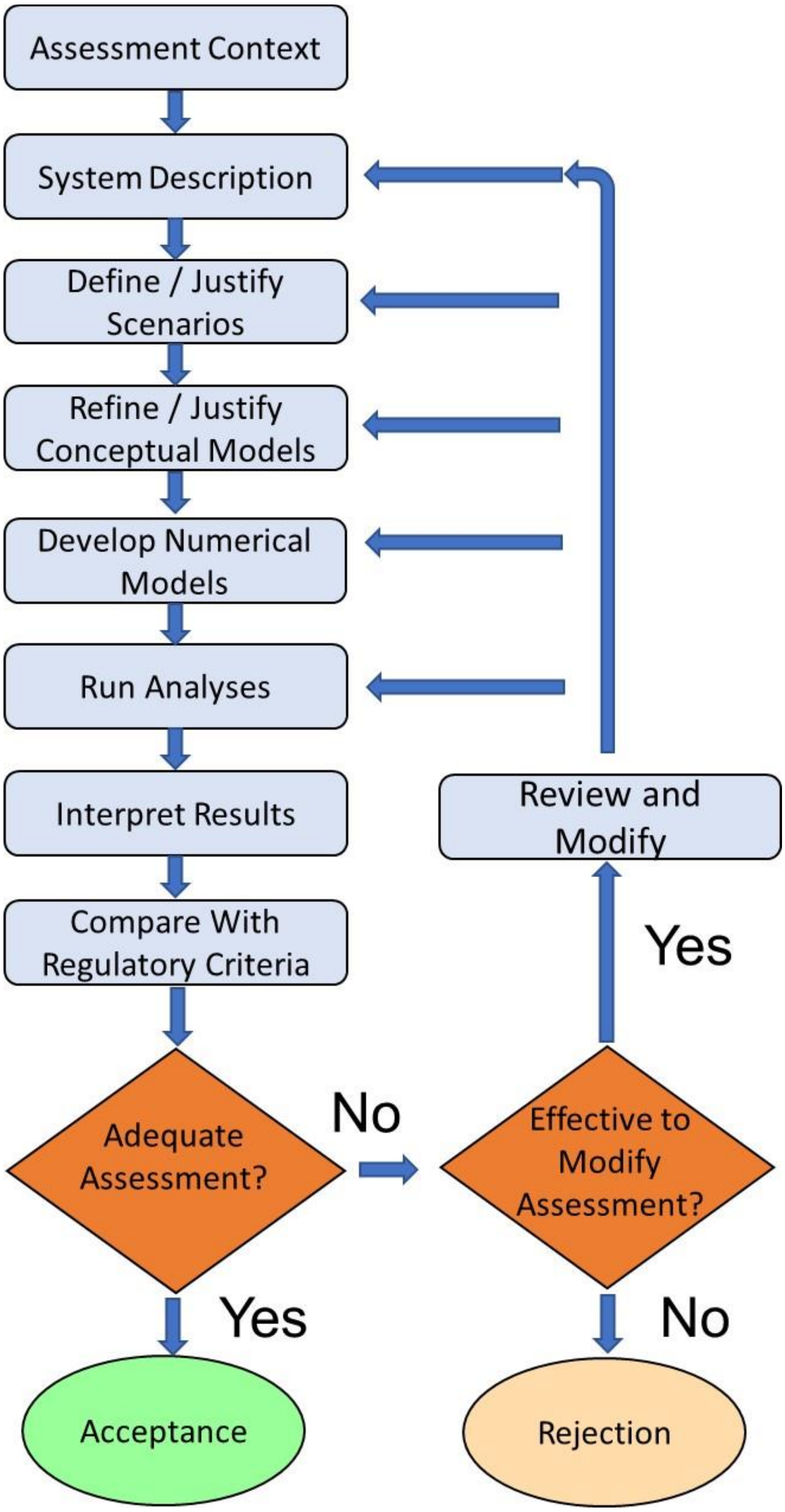


Figure 1. Approach to the assessment (after IAEA, 2004).

2.2 Performance Metrics and Thresholds

Generally, a regulator will require the potential for contamination to be assessed at some specified location, a compliance point. When a risk assessment is undertaken for some subsurface activity, such as UCG, a compliance point is likely to be specified in the deepest aquifer that could potentially be exploited. Under the European Commission's Water Framework Directive (2000/60/EC), Groundwater Directive (2006/118/EC), and Water Quality Standards Directive (2008/105/EC), an Environmental Quality Standard (EQS) is not to be exceeded for a particular pollutant.

For the purpose of this work, three representative UCG contaminants were considered:

- Phenol, an example of an electrically neutral, organic contaminant which is a non-hazardous pollutant;
- Arsenic (As), an example of a redox-sensitive hazardous pollutant that is present in aqueous form as an anion; and
- Zinc (Zn), an example of a non-redox sensitive non-hazardous pollutant that is present in aqueous form as a cation.

These contaminants are also the most common UCG pollutants (e.g. Creedy et al., 2001; Sury et al, 2004; Sadasivam et al. 2020b) and have corresponding freshwater EQS of 7.7 µg/L, 50 µg/L, and 10.9 µg/L, respectively (Water Quality Standards Directive (Directive 2008/105/EC); SEPA, 2020)). It should be noted that while the use of EQS gives a reasonable basis for comparisons, regarding the hazardous pollutants such as As, it would be necessary to argue that any released levels would be undetectable and / or less than natural levels.

Other UCG contaminants could also be included in the assessment. For instance, Sury et al. (2004) specifies that, apart from the ones considered in this work, inorganic constituents such as sulphates and boron, caused by leaching of ash and thermally affected overburden, as well as soluble gases such as ammonia and hydrogen sulphide were also commonly found in UCG affected groundwater. However, those contaminants were not considered in this work due to the assumption that the gasification generally occurs within a sequence of low-permeability rocks, through which gas will not migrate very far as the operational pressures will be lower than the natural hydrostatic pressures. Additionally, dissolved ammonia will be largely in the form of neutral NH_3, or univalent ammonium (NH_4^+) and the behaviours of these species will be broadly similar to the neutral and cationic illustrative species considered in this paper respectively. Consequently, acidic, high sulphur/chlorine water that contains dissolved ammonia and leached organics is assumed not to be present in high quantities and has been neglected in this work. Nevertheless, this does not preclude the importance of considering a wide range of contaminants in a site-specific risk assessment.

2.3 General Information

The datasets presented in this work have been taken from the literature and do not represent a particular target UCG site. However, the datasets adopted in this work are likely similar to those expected to be available in the early stages of a UCG project anywhere. Their use primarily enables illustrations of the risk assessment methodology of a hypothetical UCG project. Any measured data relevant to a particular UCG project can be readily incorporated into the model presented in this work to conduct a site-specific risk assessment.

2.3.1 Geometry

In this study, it is assumed that the coal seam of interest for UCG lies at a depth of 1,000 m below the ground surface and has a thickness of 10 m. This is based on the general recommendation that UCG should be undertaken in coal seams deeper than 300 m and not more than 2000 m to ensure sufficient containment pressure from surrounding groundwaters and maximise the calorific value of the produced gas (e.g. Yang et al., 2016). Coals at such depths are commonly found in Europe and Canada (Perkins, 2018; An et al., 2021a). However, UCG has been commonly conducted in coal seams shallower than 300 m, predominantly in China, Australia and the US (Perkins, 2018).

The distance between the injection and production wells is assumed to be 10 m and the length of the panel is 1,000 m, taking into account that the method applied is a Parallel Controlled Retracting Injection Point (P-CRIP) method (Figure 2).

A range of well diameters have been used in UCG trials up to date, ranging between 11 cm and 30 cm (Perkins, 2018). For this work, well and casing diameters of 30 cm and 25 cm have been adopted, based on the European El Tremedal UCG trial (Green, 1999).

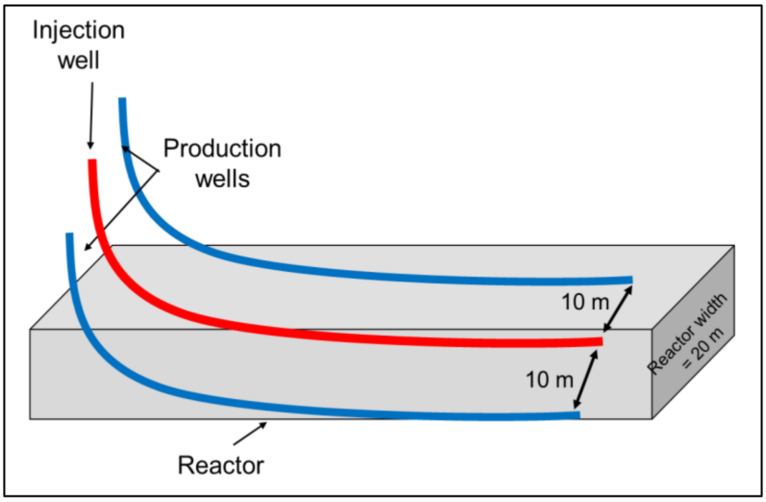


Figure 2. Schematic illustration of the P-CRIP UCG geometry.

2.3.2 Source Term

The source term for pollutants is the UCG cavity and its contained materials, such as char, ash, spalled rocks, and groundwater (Creedy et al., 2001; Sury et al, 2004; Sadasivam et al. 2020). For assessing long-term environmental impacts, the contaminants that remain in the cavity after UCG are of principal importance. The approach taken in this assessment is to specify maximum aqueous concentrations of phenol, arsenic, and zinc, and to explore the significance of those contaminants being transported to receptors via all plausible pathways. Pyrolysis and cavity pressurisation immediately post-gasification are not considered, as the cooling and re-saturation of the cavity occurs fast (e.g. Sarhosis et al. 2013) compared to the assessment time considered here.

2.3.3 Cavity Collapse

Collapse of voids created by the UCG process will create a disturbed zone (goaf) in the geological strata overlying the exploited coal seam (Perkins, 2018). The deformational stratification above a collapsed void is reflected in the development of distinct zones of permeability, similar to that of longwall mining operations (Younger, 2011). The disturbed zone, including caved and fractured zones above the mined coal seam, ranges from 6.5 to 24 times and from 11.5 to 46.5 times the extraction coal seam height in short and long terms, respectively (Majdi et al., 2012). Similarly, Younger (2011) suggests a range of 15 to 60 times the coal seam height. The exact timing, rate and size of collapse will depend on a number of different factors, such as the size of the cavity, mechanical strength of the rocks surrounding the cavity, number of panels, stress state of the rocks, and hydrostatic pressure within the cavity (Majdi et al., 2012).

For this assessment, the collapse results in a redistribution of void space, such that the net effect is for the porosity and permeability of the roof rocks to increase. In this situation, there is no driving force exerted on the fluid in the cavity due to roof collapse.

2.3.4 Parameters

Concentrations of contaminants in water and in solid constituents (ash, char) within the cavity produced by UCG are given in Table 1. The values in solid constituents are used to ensure the total contaminants released from the source zone can never exceed the total initially in the inventory, assuming constant concentrations of mobile contaminants.

Table 1. Concentrations of contaminants in cavity water and solid UCG residues.

Contaminants	Concentration in cavity water (mg/L)	Concentration in solid constituents present in the cavity (mg/kg)	Rationale
Phenols	15	Values not reported. Hence, treated as being effectively unlimited.	Sadasivam et al. (2020b)
As	0.02	23	Sadasivam et al. (2020b)
Zn	0.5	46	Sadasivam et al. (2020b)

The transport properties of the UCG cavity materials and rock formations are shown in Table 2. Sorption parameters and diffusivities of contaminants are given in Table 3 and Table 4, respectively.

Table 2. Transport properties for the coal, goaf and rock formations around a UCG cavity.

Material	Parameter	Value	Units	Rationale
Coal	Permeability	1E-15	m^2	Zagorščak and Thomas (2016)
	Porosity	0.04	-	Meng et al. (2015)
	Density	1375	kg/m^3	Zagorščak and Thomas (2018)
Goaf	Permeability	1E-11	m^2	Younger (2011)
	Porosity	0.2	-	Wang et al. (2018)
	Density	1800	kg/m^3	Assumed as 80% of density of aquiclude
Aquifers (sandstones, limestones)	Permeability	1E-14	m^2	Metcalfe et al. (2015)
	Porosity	0.3	-	Metcalfe et al. (2015)
	Density	2475	kg/m^3	Lintao et al. (2017)
Aquicludes (mudstones, shales)	Permeability	1E-17	m^2	Metcalfe et al. (2015)
	Porosity	0.1	-	Metcalfe et al. (2015)
	Density	2250	kg/m^3	Metcalfe et al. (2015)

Table 3. Sorption parameters for contaminants.

Contaminants	Sorption Coefficient m^3/kg			Rationale
	Coal Seams	Aquifers	Aquitards	
Phenols	5.0E-06	No sorption	No sorption	Kd calculated based on data in Strugała-Wilczek et al. (2021).

Contaminants	Sorption Coefficient m³/kg			Rationale
As	2.0E-01	2.0E-01	2.0E-01	USEPA (2005).
Zn	5.0E-01	2.0E-02	3.0E-02	Coal value appropriate for organic-rich soil in the absence of other data (IAEA, 2010). Aquifer value for sediment (Kaplan, 2016). Aquitard value lowest value for sediments quoted by USEPA (2005).

Table 4. Diffusivities of contaminants.

Contaminants	Diffusivity (m²/s)			Rationale
	UCG Cavity/ Coal	**Aquiclude (Mudrock)**	**Aquifer (Sandstone)**	
Phenol	1.0E-09	1.0E-12	1.0E-10	Diffusivity in coal from An et al. (2021a,b) Diffusivity in aquiclude from Dowle et al. (2019). Diffusivity in aquifer an order of magnitude smaller than in the cavity (c.f. values for neutral tracers in the Sherwood Sandstone Group in Tellam and Barker, 2006).
As	1.0E-09	1.0E-12	1.0E-10	Values as for phenol.
Zn	1.0E-09	1.0E-12	1.0E-10	Values as for phenol.

For the purposes of this illustrative risk assessment, a horizontal gradient of 0.01 is applied across all formations. This value is based on the observation that in the South Wales coalfield, the piezometric surface is much flatter than the topography, and corresponds to the valley bottoms (Robins et al., 2008).

To represent the cavity collapse, a range of parameters have been considered (Table 5).

Table 5. Parameter ranges for the cavity collapse.

Property	Units	Value		Rationale
		Minimum	Maximum	
Thickness of zone of enhanced permeability above the cavity	x coal bed thickness	15	60	Younger (2011)
Hydraulic conductivity of the zone of enhanced permeability above the cavity	m/s	1.12E-5	1.16E-3	Younger (2011)
Porosity of the zone of enhanced permeability above the cavity	-	0.2	0.3	Lower value from Wang et al. (2018), upper value from Metcalfe et al. (2015)
Diffusivity of the zone of enhanced permeability above the cavity	m²/s	8.60E-10	1.00E-9	Lower value from An et al. (2021a,b), upper value same as for phenol in goaf.
Hydrostatic head in cavity	m	1000	2700	Lower value hydrostatic, upper value lithostatic

2.4 Scenarios

Internationally, scenario analysis is often used in risk assessments for disposal, storage or use of materials underground (e.g. IAEA, 2004; NEA, 2016; NETL, 2017). In this assessment, a set of generic scenarios is specified comprising a Reference Scenario (RS) and a series of Alternative Scenarios (AS). The RS is a general description of an expected evolution for a UCG site, and risk analyses based on it, are intended as a basis for comparing the AS that describe sites with different or potentially unfavourable characteristics and events.

The International Energy Agency's Greenhouse Gas Programme (IEAGHG, 2021) identifies features, events and processes (FEP) databases as tools for auditing risk scenarios for projects to store CO_2 in the sub-surface. Features are tangible physical characteristics of a storage system, such as a storage reservoir or an injection well. Processes are dynamic changes in features, including interactions between features, that act over the entire assessment timescale, or a substantial part of it. For example, groundwater flow is a process because it will occur to some extent throughout the assessment time period. Events, in contrast, are processes that operate over very short periods compared to the assessment time frame, such as cavern collapse. A similar FEP approach is here applied to a generic UCG system, with the key FEPs based on Creedy et al. (2001), Beath et al. (2004), Younger (2011), Sarhosis et al. (2017) and Perkins (2018).

The UCG system is considered to comprise:

- Subsurface engineered components associated with UCG;
- Fluids injected into the subsurface and produced from the subsurface;
- A subsurface rock sequence, including the exploited coal seam;
- Natural subsurface fluids;
- The surface environment.

Consideration is given only to system FEPs that are consistent with the assessment context, and the focus of this work is on post-abandonment risks.

The main features of the RS are presented in Table 6 and illustrated schematically in Figure 3. The main assumptions in the development phase (Figure 3a) are that the well geometry reflects the P-CRIP method and that the casings and cement bonds are robust with respect to the injected and produced gases, while providing effective barriers to inter-formational fluid flow. During the operational phase (Figure 3b), components of the UCG system are not compromised by the in-situ gasification. As expected, minor quantities of water flow into the UCG reactor to support the gasification, but no large-scale cross-formational water flow or fault-reactivation is induced. Once the gasification is terminated (Figure 3c), UCG by-products are contained within the gasification cavity and can only migrate via diffusion. Although the subsidence of the roof of the cavity is assumed to occur, this does not result in creation of fluid flow paths through the overburden. All wells have plugs installed following best practice to prevent inter-formational flow.

The alternative scenarios are only developed for the post-abandonment phase of the UCG evolution (Table 7).

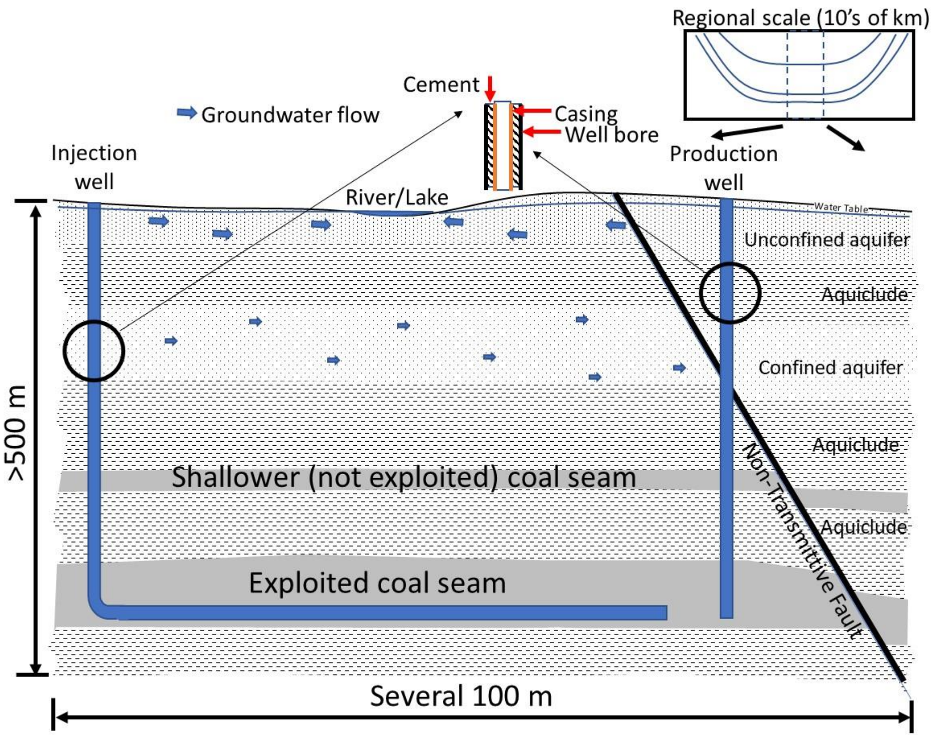
Table 6. Main features of the Reference Scenario.

Phase	Features
Site Characteristics	Coal gasification is carried out in a horizontal coal seam, within a rock sequence of horizontal sedimentary rocks. The outcrops are sufficiently far away that they need not be considered as possible discharge sites
	Rock strata surrounding the coal seams are of low permeability, within which water and solutes can move only by diffusion
	There are two aquifers, a relatively deep confined one and a shallow unconfined one, in which groundwater flows are topographically driven
	Existing faults are not hydraulically conductive, and there is no underground mine workings present
Development Phase	Well completion is conducted in line with best practice.
	Coal gasification proceeds in accordance with predictions

Phase	Features
Operational Phase	The integrity of rock formations above the target seam is not compromised, and no gaseous or dissolved chemicals escape the reactor
	Well sealing material maintains integrity, and any faults in the reactor vicinity behave as barriers to fluid flow
	Small quantities of water flow into the reactor, but these are insufficient to require large-scale cross-formational water flow
Post-abandonment Phase	Wells are abandoned in line with best practice. Cement plugs extend across all aquicludes in the geological sequence above the exploited coal seam.
	Subsidence of the roof above the UCG cavity does not result in fluid paths through the overburden. The subsidence results in the formation of a pressure arch in the overburden that is a zone of low permeability. There is no variation to surface topography due to subsidence.
	Contaminants from the UCG process remain within the char and ash in the cavity, and may leave the cavity by diffusion into the surrounding formations only

Table 7. Main features of the Alternative Scenarios.

Alternative Scenarios	Features
Inclined strata	As for the RS, but with uniformly dipping strata extending to the surface
Failed well seals	Well seals fail, providing pathways between the exploited coal seams, the aquifers and/or ground surface
Void collapse	The void above the UCG cavity is larger and/or more unstable than expected, and can include the formation of pathways between the UCG cavity, aquifers and possibly the ground surface
Conductive fault	Existing faults are more conductive than expected, that potentially form pathways between the UCG cavity, aquifers and possibly the ground surface
Adjacent underground human activities	Past, present or future human subsurface activities near the UCG site cause leakage pathways. This could include disused and/or new mine workings, groundwater abstractions, hydrocarbon exploitation, underground storage of fluids



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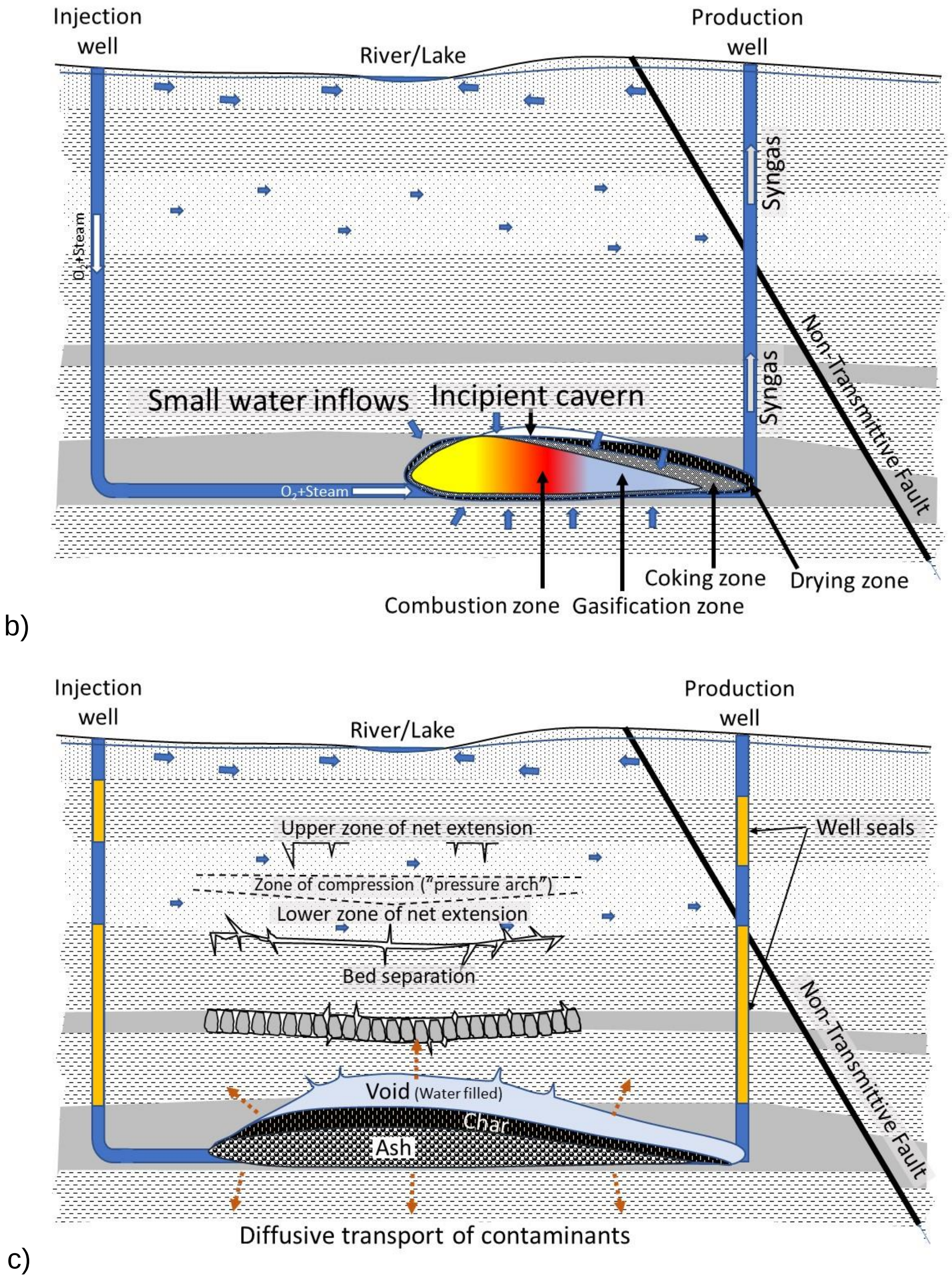

Figure 3. Reference Scenario: a) Implementation phase; b) Operational phase; c) Post-abandonment phase.

3 Model Development

3.1 Software

The numerical models that are used to explore the post-abandonment environmental performance of the UCG system are implemented in the AMBER 6.4 software package. AMBER is a compartment modelling tool that has been widely used for a wide range of risk assessments (Quintessa, 2019a,b). AMBER has been extensively tested against a broad set of verification and validation tests (Quintessa, 2019c).

The software allows a user to represent a system of interest as a collection of any number of compartments and represent the migration, degradation and fate of contaminants in environmental system, as appropriate for the assessment. Generally, each compartment represents all or part of a system component. The user can specify equations governing the behaviour of contaminants within each compartment and contaminant transfers between the compartments. Time-varying parameter values can be specified. Equations and data are defined as AMBER parameters which, with information on the model structure, are saved in text-based case files which allow easy checking of the model. Output of results and data can be made directly to Microsoft Excel in files stamped with the date and model filename. This ensures that the Quality Assurance of results is very efficient.

3.2 Conceptual Model

This section describes the simple conceptual models derived from those scenarios that are used to describe the post-abandonment evolution. The conceptual model descriptions include details of the conceptual-level simplifications that are appropriate for the assessment of risks at high level. While the model assumptions are simple, the parameters used in the models take account of available underpinning information and analysis to allow the more detailed understanding to be represented implicitly in the simplified model.

3.2.1 Reference Scenario (RS)

At the end of the gasification process, the hot cavity is filled with gaseous species and is expected to resaturate on a timescale of a few months to a few years (Sarhosis et al., 2013). Hence, the resaturation time is likely to be comparable with the timescale on which the injection and production wells would be sealed and small compared with the overall timescales considered in the assessment. In the calculations reported here, the time to full resaturation is specified to be a maximum of two years (e.g. Sarhosis et al., 2013).

It is assumed that collapse of the overlying strata into the void happens relatively quickly, as is observed during longwall mining. For the RS, thickness of damaged zone above the UCG cavity is 100 m.

Degradation of some contaminants is likely to be rapid compared to the assessment timeframe (e.g. Sadasivam et al., 2020b), however it is conservative to assume no degradation, as it maximises the calculated concentrations of these contaminants in the receptors. Hence, the calculations do not include contaminant degradation.

In the RS, the coal seam does not crop out at the surface. Therefore, flow along the coal seam could not result in contamination reaching the surface unless the coal seam is connected to the surface by transmissive features such as faults and / or other strata that crop out (e.g. if the coal is unconformably overlain by an aquifer some distance from the UCG site), or if there are un-/poorly sealed boreholes / wells. In the RS, it is assumed that such pathways do not occur. None of the other potential pathways are expected to contribute to contaminant migration because the well seals are all expected to perform as designed and any faults that cut the sequence are not transmissive. Were any contamination to reach one of the overlying aquifers it would be diluted on entry and then the concentration would be further diluted and dispersed during advective transport.

3.2.2 Inclined Strata Scenario (AS1)

In this scenario, the coal seams dip such that the coal seam within which UCG is carried out extends to the surface. This exploited coal seam could provide a pathway to the surface if it is transmissive and there is a driving force for flow along it.

All the processes described for the RS apply for this scenario. Advective transport along the coal seam is significantly enhanced relative to the RS where it is negligible. Advective transport through the coal seam requires the seam to be sufficiently transmissive and for there to be a large enough head gradient to drive flow. One, albeit unlikely, situation that could result in advective flow is the case in which the coal bed is part of a syncline and crops out both upstream and downstream of the source zone so that flow is driven by recharge and topographic differences between the two outcrop locations. It seems unlikely that significant topographic driving gradients would penetrate to depths of 1000 m or more in the areas that typically host coal fields. Therefore, scenarios in which the coal seam crops out at the surface are unlikely to also include significant advective flow along the coal seam unless the upstream end of the coal seam has a good connection to a region of high head and a source of water. This type of connection in turn implies that one or more of the other AS, for example conductive faults or connections via manmade structures such as mine workings or wells is also occurring.

3.2.3 Failed Well Seals (AS2)

In this scenario some or all the seals in the injection well and the production well fail, providing pathways between the exploited coal seam, the aquifers and/or the ground surface. This scenario bounds all scenarios for poorly sealed or unsealed wells because the wells are considered have a direct connection to the source zone.

Wells add the potential to bypass the barriers that are provided by the low permeability aquiclude units. The extent to which this occurs depends on the locations of the failed seals and the extent to which they have failed. Advective flow would probably be required for the connection to be significant for contaminant transport because the small cross-sectional area of the well would limit the diffusive flux even if the diffusivity is high. Advective flow will be driven by head differences between the various layers or, at early times, temperature and therefore density differences between the hot source zone and the cooler rocks above.

If the seal between the source zone and the deepest aquifer fails before the roof of the source zone collapses, the collapse episode could result in contaminated water being pushed directly into the aquifer. This event would likely occur while the source zone was still warm and while contaminant concentrations are still high.

In the unlikely event of the seal between the source zone and the lower aquifer failing in more than one well, there is the potential for water to flow down one well, through the source zone and then up the other well. Such a scenario would be dependent on local head conditions, and it is noted that the injection and production wells are assumed to be separated by a maximum of 20 m meaning that the driving head for such a flow would likely be very small.

3.2.4 Void Collapse (AS3)

In this scenario, the void above the site of coal gasification is larger and/or more unstable than expected, resulting in greater deformation of the overburden than anticipated. This deformation can include the formation of pathways between the site of coal gasification, one or both aquifers in the overburden, and possibly the ground surface (though this latter is unlikely given the great depth of the UCG cavity).

This scenario has the potential for significantly increased vertical transport of contaminants compared with the RS. Advective flow between the source zone and the lower aquifer is possible both during the collapse event and in the longer term if local head gradients drive such flow and there is sufficient permeability in the coal seam to provide the water. If the distance between the source zone and lower aquifer is small, the source zone could locally become part of the aquifer (i.e. the aquifer thickness is locally increased) allowing direct flow through the source zone. Diffusion between the lower shallower aquifers is also enhanced because of the rock being damaged even if conditions are not suitable for an advective pathway to develop.

The timing of void collapse relative to resaturation is especially important for this scenario because contaminated water that is expelled from the source zone could potentially reach the lower, confined aquifer during the collapse event.

3.2.5 Conductive Fault (AS4)

In this scenario, there is a fault that is more conductive than expected, that could potentially form a pathway between the site of coal gasification, one or both aquifers in the overburden, and possibly the ground surface.

Unlike the wells considered in AS2, the fault would not directly intersect the source zone. A conductive fault can act as a pathway between geological formations, for example between aquifers. Transport may be by advection or diffusion, depending on the prevailing head gradients. Transport via a fault may result in larger fluxes of contaminant than transport via wells due to the larger cross-sectional area of the fault (i.e. it is longer and wider).

3.2.6 Adjacent Underground Human Activities (AS5)

Past, present or future human activities, such as mining, groundwater abstractions, hydrocarbon exploitation, or underground storage of fluids in underground spaces near to the site of coal gasification may cause pathways to form between the site of coal gasification, one or both aquifers in the overburden, and possibly the ground surface.

However, AS5 is not analysed using a numerical model as the consequences of AS5 would likely be bracketed by the consequences of the other AS. Furthermore, as a range of human activities can be envisaged, each of which would be very site-specific, any numerical analysis of AS5 would be speculative.

3.3 Mathematical Model

3.3.1 Spatial Representation and Discretisation

A generic mathematical model has been constructed to represent the conceptual models. The basic geometry of the model components is shown in Figure 4. There are three components to the source zone, which is overlain by a collapse zone. Once resaturation and collapse have occurred, it is assumed that the contaminant concentrations will be uniform throughout the zone that comprises the original gasification chamber (ash, char, goaf and void) and the collapsed roof rock. The volume and hydrogeological properties (primarily porosity) of the source zone will depend on the extent of collapse.

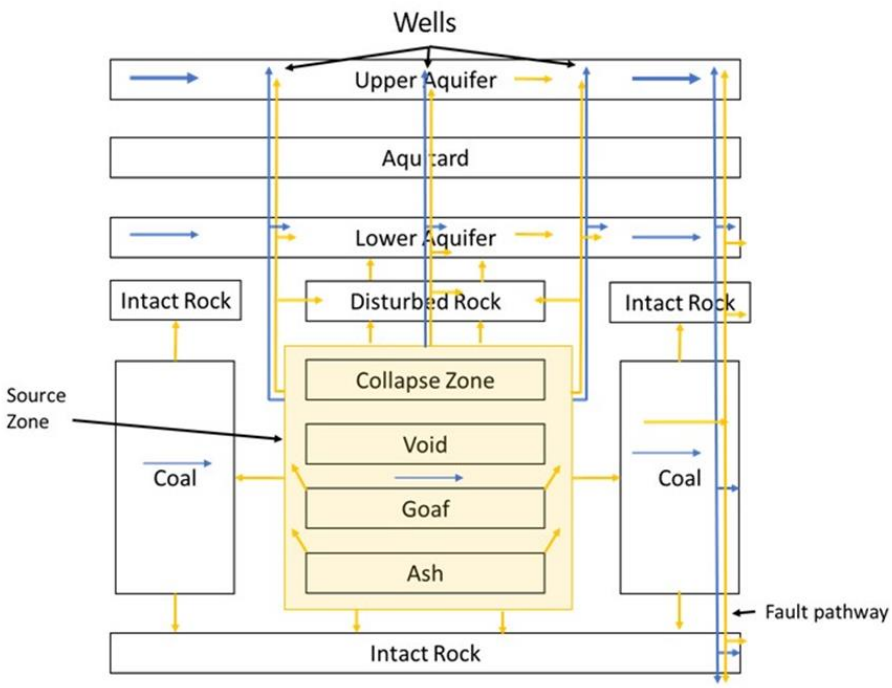

Figure 4. Schematic showing the model components. Blue arrows indicate possible water flows and orange arrows indicate possible contaminant movements.

The approach is to develop a model of a single UCG panel that can be used to carry out scoping calculations to explore the extent to which contaminants can move between the source (UCG cavity) and receptors (a shallower coal seam or aquifer). The single panel model is flexible and allows the implemented processes to be turned on and off to explore different aspects of the system (e.g. the implications of advective contaminant transport or diffusive transport). The model can also be parameterised as required to explore uncertainties.

The single panel model represents a single UCG chamber and half a pillar width either side of that chamber for the full length of the panel. The 1 km long panel is split into five lengths of 200 m each. To give some representation of the migration of contaminants into the pillar, the pillar sections are represented using two compartments for each length of panel considered (Figure 5). The widths of the compartment sections are shown in Figure 6.

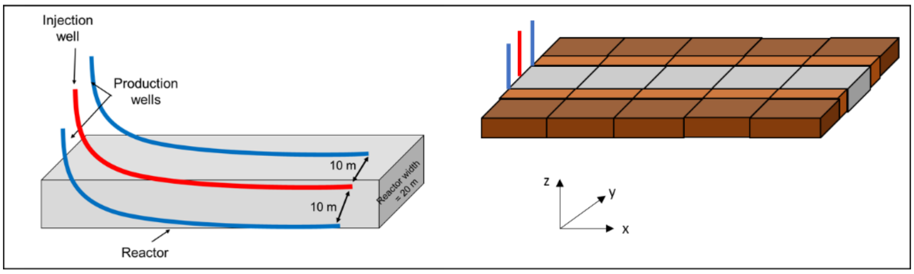

Figure 5. Schematic of the discretisation of the UCG layer for the single panel model.

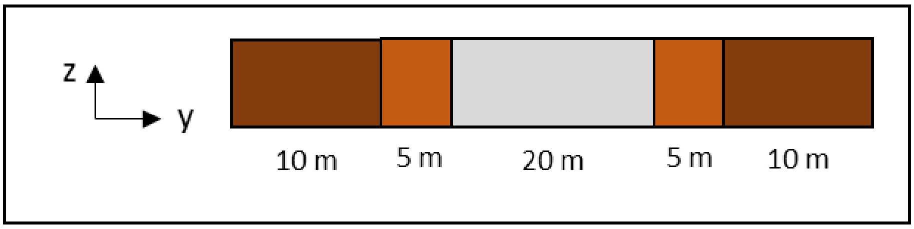

Figure 6. Widths of compartment sections in the single panel model in the Y-Z plane.

The discretisation established for the UCG layer is then propagated throughout the overlying geosphere (Figure 7). The aquiclude regions are each split into five vertical layers, to adequately represent diffusion processes (Quintessa, 2019b). The aquifer regions are split into two layers vertically, to better represent the mixing in those regions. These columns are replicated in the X-Z plane also. The single panel UCG system is therefore represented using 525 cells.

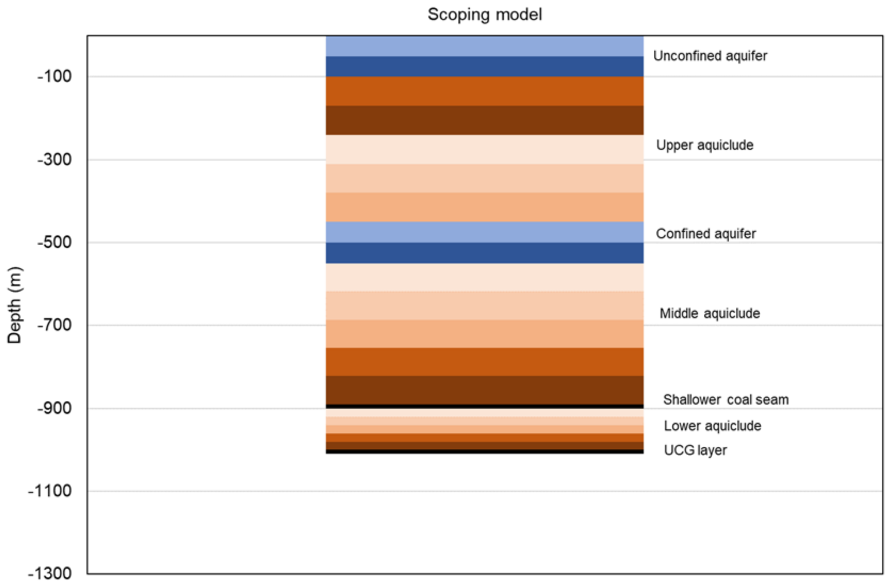

Figure 7. Vertical discretisation of the single panel system in the Z-axis. Each layer is split into compartments as shown in Figure 6. Black indicates coal seams; blue indicates aquifers; and brown indicates aquicludes. Different shades of each colour indicate different compartments.

3.3.2 Source Term

The contaminants are initially present primarily in the ash and char, though certain contaminants will also be present in the goaf, as they occur naturally in the rocks. Contaminants are assumed to be capable of dissolving in water as soon as the ash and goaf are contacted by water, and to mix freely with water in the void. It is assumed that there are no mobile non-aqueous phase liquids.

In the numerical model of the source term (UCG cavity):

i. The entire contaminant inventory in the UCG cavity is available for dissolution in the aqueous phase;

ii. The aqueous contaminants can sorb to solid phase surfaces;

iii. The aqueous concentrations of the contaminants are held constant, i.e. treated as being solubility-limited. The solubility limitation will apply until the solid phase (or non-aqueous liquid phase) is depleted. Thereafter, the concentration of the contaminant will decrease owing to dilution by groundwater entering the cavity and continued transport out of the cavity.

3.3.3 Pathways

Potential pathways that are represented in the mathematical model are:

i. Diffusion through the roof of the UCG cavity;

ii. Permeable strata, including the exploited coal seam and aquifers in the overburden;

iii. A column of rubble and fractured rock, produced by collapse of the UCG cavity roof;

iv. Wells with failed seals;

v. Transmissive faults.

Which of these pathways is/are active depends on the scenario considered. Accordingly, the model allows these different pathways to be switched on and off as required. Transfers of contaminants between components will be by advection or diffusion (or a combination of the two). Table 8 summarises the characteristics of the various transfers shown in Figure 4.

Table 8. Contaminant transfer types for volume outside source zone. Transfers in all scenarios are the same as the Reference Scenario, unless stated (AS3 differs from the Reference only by having a higher collapse zone; transfers are the same).

Transfer	Scenario	Transfer Type
Source Zone (UCG cavity) to Coal	Reference	Low advective flux in coal: diffusion
	AS 1	Higher flow rate in coal: advective component in downstream transfer
Source Zone to Intact Rock below	Reference	Diffusion
Source Zone to Disturbed Rock	Reference	Diffusion Advection if vertical head gradient present
Coal to Intact Rock	Reference	Diffusion both upwards and downwards
Within Coal	Reference	Low advective flux in coal: diffusion
	AS 1	Higher flow rate in coal: advective component in downstream transfer
Intact Rock to Lower Aquifer	Reference	Diffusion both upwards and downwards
Within Intact Rock	Reference	Diffusion both upwards and downwards
Disturbed Rock to Lower Aquifer	Reference	Diffusion both upwards and downwards Advection if vertical head gradient present
Within Disturbed Rock	Reference	Diffusion If vertical head gradient present, advective flux up through the disturbed rock
Within Lower Aquifer	Reference	Advection and diffusion
Lower Aquifer to Aquiclude	Reference	Diffusion both upwards and downwards
Within Aquiclude	Reference	Diffusion both upwards and downwards
Aquiclude to Upper Aquifer	Reference	Diffusion both upwards and downwards
Within Upper Aquifer	Reference	Advection and diffusion
Source Zone to Well	AS 2	Diffusion Advection if vertical head gradient present
Well to Lower Aquifer	AS 2	Diffusion If vertical head gradient present, advection could bypass the Lower Aquifer, depending on where the seals in the well fails (e.g. if there is casing across the lower aquifer and a failed well seal within the casing).

Transfer	Scenario	Transfer Type
Well to Upper Aquifer	AS 2	Diffusion Advection if vertical head gradient present
Well to Aquiclude	AS 2	Negligible – not included
Coal to Fault	AS 4	Advection and Diffusion (if close enough to source for diffusion to be considered)
Fault to Intact Rock	AS 4	Advection, if vertical head gradient present, and Diffusion (close enough to source for diffusion to be considered)
Fault to Lower Aquifer	AS 4	Advection if vertical head gradient present; Diffusion if advection negligible
Fault to Aquiclude	AS 4	Diffusion
Fault to Upper Aquifer	AS 4	Advection if vertical head gradient present; Diffusion if advection negligible

Advective transfers are described by:

$$\lambda = \frac{Q_{adv}}{V\phi R} \quad (1)$$

where λ (/y) is the transfer rate, Q_{adv} is the advective flux (m^3/y) V is the volume of the donor compartment (m^3), ϕ is the porosity of the compartment (-) and R is the retardation factor (-):

$$R = 1 + \frac{\rho K_d}{\phi} \quad (2)$$

where ρ is the dry bulk density of the material (kg/m^3) and K_d is the sorption coefficient (m^3/kg). Q_{adv} is determined from the overall understanding of the hydrogeology. For the advective transfers associated with void collapse Q_{adv} is determined by considering the change in the volume of the source zone because of the subsidence of the overlying formation, the development of enhanced porosity within it and the time over which the collapse happens.

Diffusive transfers are described by:

$$\lambda = \frac{D_{eff}\ A}{V\phi R\Delta} \quad (3)$$

where D_{eff} (m^2/s) is the effective diffusion coefficient, A is the area over which the diffusion is occurring (m^2) and Δ is the distance between the mid points of the two compartments over which diffusion is occurring (m).

In calculation cases that include some roof collapse, the porosity of the layers affected is modelled as a thickness weighted average of the porosity of the layers prior to the roof collapse.

$$\phi_{CollapseZone} = \frac{\sum_j \phi_j Z_j}{\sum_j Z_j} \quad (4)$$

3.3.4 Receptors

In this model two aquifers, labelled “Lower Aquifer” and “Upper Aquifer” in Figure 4 are the potential receptors of interest. It is likely that the former will be of primary interest to regulators, since generally they will specify a compliance point in the deepest groundwater aquifer, whether or not it can be exploited for water resources; in practice many deep aquifers will contain groundwater too saline for exploitation. However, it may be that stakeholders are interested in the shallower, Upper Aquifer, representing an unconfined aquifer. In some sites there may only be an unconfined aquifer and / or surface water bodies, which can be represented by the Upper Aquifer. The model has been designed to represent these different situations flexibly.

Because this paper presents and illustrates a risk assessment methodology, rather than anactual risk assessment "evaluation point" is used in place of "compliance point" in the following sections.

3.3.5 Parameters Exploration

The key aspects associated with the potential migration of contaminants from the UCG cavity are explored and shown in Table 9. The details of all the cases are given in the Appendix. Inevitably values of parameters could vary considerably between different sites, reflecting both site-specific geological and hydrogeological factors and project-specific design factors. Hence, the purpose of the calculations presented here is to understand and illustrate the sensitivities of contaminant concentrations at key points in the modelled system to process couplings. Therefore, the requirement is to use plausible parameter values for the base case of the RS analysis, and then to vary these parameter values by plausible ranges.

Table 9. Summary of the key aspects investigated in each scenario.

Scenario	Key aspects
Reference Scenario (RS)	Time of collapse of overlaying rock into void versus resaturation extent and time. The potential significance of an upwards head gradient.
Inclined Strata (AS1)	Flow occurs through inclined strata towards the ground surface. A range of flow rates through the coal are considered. In this case, the coal seam that is exploited for UCG, or the one above it, act as pathways for the transport of contaminants.
Failed Well Seals (AS2)	The pathways associated with the wells are activated. Cases considered involve direct flow from the source zone to one or more layers. Timing of well failure, and the presence of a vertical hydraulic gradient are considered.
Void Collapse (AS3)	Extensive damage to the rock above the source zone. The AS3 case in which the collapse zone just reaches the lower aquifer is therefore used as the basis for exploring the impact of changes to the properties of the hydrogeological units and the contaminant transport properties.
Conductive fault (AS4)	Connections associated with the fault are activated. Both upwards and downwards flow is considered. Calculations consider both very low flow in the coal (diffusion dominated) and more significant flow from the coal into the fault, with the fault located 100 m downstream from the source zone.

4 Results and Discussion

A suite of calculations has been undertaken to explore the behaviour of the RS and to explore the possible impact of the AS on system behaviour. These calculations aim to understand which processes and parameters are the most important for determining system behaviour. To meet this goal, it was necessary to implement only a small number of model cases, each one representing a different combination of processes and / or parameter values. For a risk assessment applied to a real site to support a permit application, it would be necessary to carry out many more calculations to explore system behaviour and uncertainties more fully. In many cases, parameter values are highly uncertain and therefore plausible values, based on published literature, have been used.

The key outputs of interest are the concentrations of contaminant in the aquifer compartments and those immediately below them, and the fluxes of contaminants into the aquifer compartments.

In addition to concentrations within the system itself, consideration is given to concentrations of contaminants in different locations downstream in the coal seam that has been exploited by UCG and the shallower coal seam. These concentrations are reported 1, 5 and 10 km downstream of the UCG site.

4.1 Reference Scenario (RS)

The parameters explored when analysing this scenario relate to the duration of the UCG cavity roof collapse and its timing relative to resaturation. Cases were run for roof collapses lasting for 1, 10, 50 and 100 years, but roof collapse extends only 100 m above the gasified coal seam.

The calculated concentrations of all three contaminants in the lower, confined aquifer increase over time, the maximum values being reached at the end of the 10,000-year calculation period in all cases. However, calculated contaminant concentrations are extremely small, far below any level that could reasonably be detected (which practically is likely to be > 1E-3 µg/L and possibly significantly greater than this value). Calculated concentrations of phenol are more than 10 orders of magnitude lower than the surface freshwater EQS of 7.7 µg/L, and the maximum calculated concentrations of both As and Zn, which are both assumed to be retarded in the aquiclude and coal layers, are more than 38 orders of magnitude below the relevant surface freshwater EQS.

The concentrations of contaminants in the UCG cavity are conservatively held at constant values. Thus, over time they diffuse through the intact rock above the collapse column and enter the deep aquifer. Assuming that the water flux in the aquifer is constant, given long enough, the concentrations in the aquifer would attain a steady state. If the water in the aquifer were to be stagnant then eventually the concentrations in the aquifer would approach the same values as in the UCG cavity. However, a flux of water within the aquifer, driven by the natural head gradient, would dilute the contaminants. The attainment of a steady state will require a time scale many orders of magnitude longer than the calculation period of 10,000 years.

Overall, in the RS, roof collapse of the UCG cavity does not break through to the aquifer. Hence, there is always a substantial thickness of aquiclude above the collapsed column. Contaminant transport through this intact roof is by diffusion, which is a very slow process.

4.2 Inclined Strata Scenario (AS1)

In this scenario consideration has been given to advective lateral groundwater flow in the coal seams both with (AS1-1 and AS1-2) and without (AS1-3 to AS1-7) 100 m of roof collapse. Results are summarised in Table 10 and Table 11 for the deeper coal seam in which UCG is carried out and for the shallower coal seam, respectively.

Concentrations of contaminants decrease downstream from the UCG cavity, due to longitudinal dispersion (mixing with water already present downstream) and sorption in the coal seam. The concentrations conservatively take no account of lateral dispersion along the flow line. However, the compartments outside the UCG cavity are large (100's m long to 1 km long; pore volume up to 8000 m^3), which means that reported concentrations are averaged over large volumes. Nevertheless, these scoping calculations indicate generally the plausible magnitude of contaminant fluxes towards the surface via an inclined coal seam.

In the upper coal seam, similar decreases in contaminant concentrations are calculated with increasing distances downstream. However, the concentrations of all contaminants at each point of interest (i.e. at 1 km, 5 km and 10 km downstream) in the upper coal seam are lower than the concentrations at the points of interest vertically below it in the coal seam with the UCG cavity. The reason for this difference is that before being transported laterally through the upper coal seam, the contaminants must be transported vertically from the lower coal seam. This transport is only diffusive owing to the lack of an upwards head gradient in any case; it occurs down a concentration gradient. Thus, the concentrations of contaminants entering the upper coal seam are lower than the concentrations in the UCG cavity.

Table 10. AS1: Calculated maximum contaminant concentrations in the lower coal seam where UCG is carried out, at the end of the UCG panel after 10,000 years, and at 1 km, 5 km and 10 km downstream (µg/L).

Contaminant	AS1-1	AS1-2	AS1-3	AS1-4	AS1-5	AS1-6	AS1-7
		Key Differences from AS1-1					
		2x head gradient	No collapse	No collapse Lower porosity	No collapse Higher porosity	No collapse Lower K	No collapse Higher K
End of UCG							
Phenol	2E+04	2E+04	2E+04	2E+04	2E+04	2E+04	2E+04
As	2E+01	2E+01	2E+01	2E+01	2E+01	2E+01	2E+01
Zn	5E+02	5E+02	5E+02	5E+02	5E+02	5E+02	5E+02
1 km from UCG							
Phenol	4E+03	8E+03	4E+03	7E+03	2E+03	6E+02	1E+04
As	2E-07	9E-07	2E-07	2E-07	2E-07	2E-08	3E-05
Zn	9E-07	4E-06	9E-07	9E-07	9E-07	9E-08	1E-04
5 km from UCG							
Phenol	2E+00	6E+01	2E+00	3E+01	3E-01	4E-03	1E+04
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
10 km from UCG							
Phenol	3E-04	8E-02	3E-04	3E-02	1E-05	2E-08	3E+03
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10

Table 11. AS1: Calculated maximum contaminant concentrations in the upper coal seam above the end of the UCG panel after 10,000 years, and at 1 km, 5 km and 10 km downstream (µg/L)

Contaminant	AS1-1	AS1-2	AS1-3	AS1-4	AS1-5	AS1-6	AS1-7
		Key Differences from AS1-1					
		2x head gradient	No collapse	No collapse Lower porosity	No collapse Higher porosity	No collapse Lower K	No collapse Higher K
End of UCG							
Phenol	2E+04	2E+04	2E+04	2E+04	2E+04	2E+04	2E+04
As	2E+01	2E+01	2E+01	2E+01	2E+01	2E+01	2E+01
Zn	5E+02	5E+02	5E+02	5E+02	5E+02	5E+02	5E+02

1 km from UCG							
Phenol	4E+03	8E+03	4E+03	7E+03	2E+03	6E+02	1E+04
As	2E-07	9E-07	2E-07	2E-07	2E-07	2E-08	3E-05
Zn	9E-07	4E-06	9E-07	9E-07	9E-07	9E-08	1E-04
5 km from UCG							
Phenol	2E+00	6E+01	2E+00	3E+01	3E-01	4E-03	1E+04
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
10 km from UCG							
Phenol	3E-04	8E-02	3E-04	3E-02	1E-05	2E-08	3E+03
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10

4.3 Well Failure Scenario (AS2)

It is assumed that the well is downstream of the UCG system with respect to the groundwater flow direction. Analyses of this scenario explore the significance of a step increase in the hydraulic conductivity and porosity in narrow features that connect the UCG cavity with the shallower coal seam; the shallower coal seam with the confined aquifer; and the confined aquifer with the unconfined aquifer. There are three key parameters of interest in this scenario: i) the time at which the well seal fails; ii) the change in hydraulic conductivity of the well seals during failure; and iii) the change in porosity.

In this scenario, consideration has been given to the effect of a well seal failure, combined with (AS2-1, AS2-2 and AS2-5) and without (AS2-3, AS2-4 and AS2-6) a 100 m roof collapse. In addition, variants AS2-5 and AS2-6 consider the presence of a vertical head gradient. Except for the phenol in cases AS2-5 and AS2-6 the calculated contaminant concentrations are well below any level that could reasonably be detected (which practically is likely to be > 1E-3 µg/L and possibly significantly greater than this value). That is, for the failed well parameters considered, only when there is an upward head gradient, such that advection can occur, is there any significant migration of any of the contaminants to the deepest aquifer via the well, after well seal failure (Table 12 and Figure 8).

The effect of assuming a vertical head such that there is upwards advective groundwater flow in both the failed well seal and also the region of void collapse, leads to a substantial increase in the maximum calculated concentrations of contaminants in the confined aquifer, but these are still several orders of magnitude below the equivalent EQS.

Although phenol concentrations are smaller than the EQS in cases AS2-5 and AS2-6, the calculated concentrations are still increasing after 10,000 years and might approach levels that conceivably could be detected. Nevertheless, as this is assumed to be an unexpected evolution scenario, which is by nature pessimistic, it is unlikely that such situation would occur and it if does, the results show that the calculated values are below EQS. Alternatively, the assessment time could be expanded to calculate the peak contaminant concentrations and demonstrate the decreasing trend.

Table 12. AS2: Effect of well seal failure on calculated maximum average concentrations of contaminants in the confined aquifer after 10,000 years (µg/L).

Averaged over the 5 deepest compartments in this aquifer, immediately above the UCG cavity.

Contaminant	AS2-1	AS2-2	AS2-3	AS2-4	AS2-5	AS2-6
		Key Differences from AS2-1				
		Later seal failure	No collapse	Higher initial seal diffusivity	Vertical head gradient	No collapse vertical head gradient
Phenol	<1E-10	<1E-10	<1E-10	<1E-10	3E-03	3E-03
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10

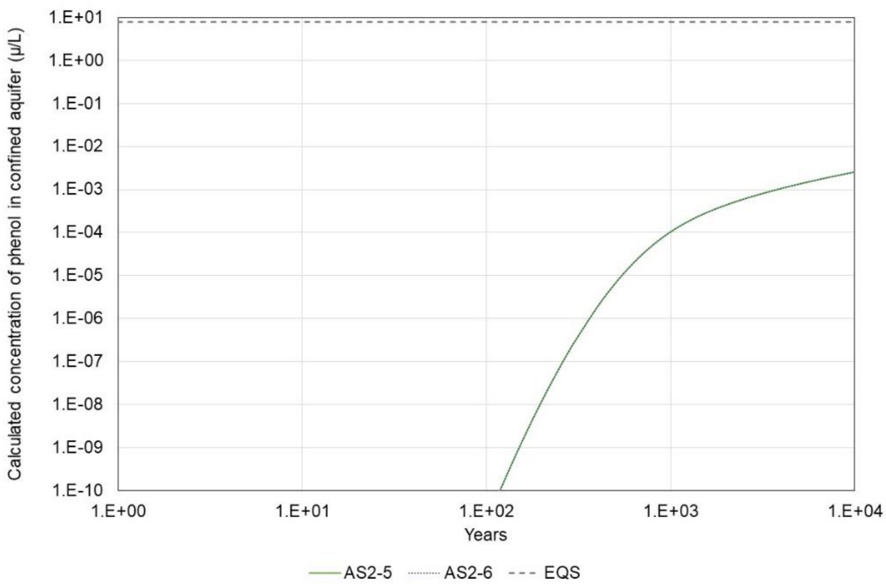

Figure 8. Calculated concentration of phenol in the confined aquifer for the AS2 scenario (µg/L). Cases AS2-5 and AS2-6 give the same curves.

4.4 Void Collapse Scenario (AS3)

This scenario considers the impact of the roof collapse being more extensive than in the RS. The thickness of the layer of rock disturbed during any collapse is assumed to be between 15 to 60 times the thickness of the UCG cavity (Younger, 2011). In the generic model the UCG cavity height is assumed to be 10 m, leading to a disturbed rock thickness of between 150 to 600 m. The roof collapse will lead to changes in hydraulic conductivity, porosity and diffusivity that affect different rock units about the UCG source zone.

The effect of assuming a more extensive roof collapse (AS3-1 to AS3-4) than the RS is a general increase in the calculated concentrations of contaminants in the confined aquifer (see Table 13 and Figure 9). Once the roof collapse is such that it breaks through to the overlying aquifer, 450 m above the site of UCG in the deeper coal seam, then the calculated concentrations of the non-retarded phenol, exceed the EQS. The phenol concentrations in cases AS3-2 and AS3-2 are still increasing after 10,000 years and might approach levels that conceivably could be detected. Similar to the AS2, the assessment time could be expanded to calculate the peak contaminant concentrations and demonstrate the decreasing trend. However, as rock collapses larger than 300 m above the cavity at 1,000 m depth are unlikely, such values present the worst-case scenarios.

Table 13. AS3: Effect of void collapse thickness on calculated maximum average concentrations of contaminants in the confined aquifer after 10,000 years (µg/L). Averaged over the 5 deepest compartments in this aquifer, immediately above the UCG cavity.

Contaminant	RS-1	AS3-1	AS3-2	AS3-3	AS3-4
	Key Differences Between Cases				
	Collapse 100 m	Collapse 150 m	Collapse 300 m	Collapse 450 m	Collapse 600 m
Phenol	<1E-10	<1E-10	2E-05	3E+02	6E+03
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10

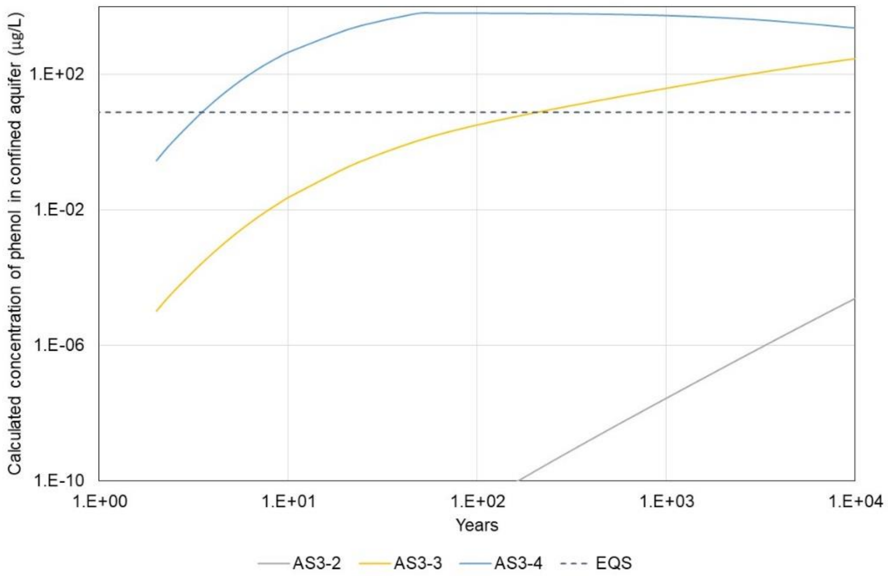

Figure 9. Calculated concentration of phenol in the confined aquifer for the AS3-2 to AS3-4 scenarios (µg/L).

The 450 m roof collapse variant calculation has then been used as a starting point to examine the effects of different assumptions regarding hydrogeological and chemical parametrisation of the system:

- Alternative hydraulic conductivities (AS3-5 to AS3-11);
- Alternative porosities (AS3-12 to AS3-16);
- Alternative effective diffusivities (AS3-17 to AS3-19);
- Alternative hydraulic gradients (AS3-20 to AS3-21); and
- Alternative sorption coefficients (AS3-22 to AS3-25).

The effect of increasing or decreasing the hydraulic conductivities is negligible on the maximum calculated concentration of the contaminants. The calculated concentrations of contaminants in the confined aquifer are also insensitive to the assumed porosity of the coal layers. However, decreasing or increasing the assumed porosity of the aquifers serves to increase or decrease, respectively, the calculated concentrations of contaminants in the confined aquifer. This is expected as porosity affects the volume available for contaminated liquid to be present in the aquifers. Increasing the assumed porosity of the aquicludes (AS3-16) serves to reduce the calculated concentrations of contaminants in the confined aquifer as there is a larger volume for contaminants to migrate through to reach the confined aquifer (Table 14).

Table 14. AS3: Effect of alternative porosities on calculated maximum average concentrations of contaminants in the confined aquifer after 10,000 years (µg/L). Averaged over the 5 deepest compartments in this aquifer, immediately above the UCG cavity.

Contaminant	AS3-3	AS3-12	AS3-13	AS3-14	AS3-15	AS3-16
		Key Differences From AS3-3				
		Porosity coal lower	Porosity coal higher	Porosity aquifer lower	Porosity aquifer higher	Porosity aquicludes higher
Phenol	3E+02	3E+02	3E+02	6E+02	2E+02	6E+01
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10

Increasing the assumed effective diffusivity in the damaged zone (AS3-17) leads to an increase in the calculated concentrations of contaminants in the confined aquifer, whereas either decreasing the effective diffusivity of the coal seams or increasing the effective diffusivity of the aquicludes has a negligible impact on the calculated concentrations of contaminants in the confined aquifer (Table 15).

Table 15. AS3: Effect of alternative diffusivities on calculated maximum average concentrations of contaminants in the confined aquifer after 10,000 years (µg/L). Average over the 5 deepest compartments in this aquifer, immediately above the UCG cavity.

Contaminant	AS3-3	AS3-17	AS3-18	AS3-19
		Key Differences From AS3-3		
		Diffusion coefficient damaged zone higher	Diffusion coefficient coal seams lower	Diffusion coefficient aquicludes higher
Phenol	3E+02	2E+03	3E+02	3E+02
As	<1E-10	<1E-10	<1E-10	<1E-10
Zn	<1E-10	<1E-10	<1E-10	<1E-10

Alternative assumptions regarding the hydraulic gradient of the system (AS3-20 and AS3-21) have a negligible impact upon the calculated maximum concentrations of contaminants in the confined aquifer. Cases AS3-22, AS3-23 and AS3-24 consider the effects of neglecting any retardation in the coal layers, aquifers and aquicludes respectively. The implications of these assumptions are negligible for phenol, which in the RS is assumed only to be sorbed in the coal layers. However, for As and Zn, both of which are assumed to be sorbed in all three types of media in the RS, disregarding sorption in any media leads to increased calculated concentrations of these contaminants in the confined aquifer (Table 16).

Table 16. AS3: Effect of alternative hydraulic gradient (AS3-20 to AS3-21) and alternative sorption coefficients (AS3-22 to AS3-24) on calculated maximum average concentrations of contaminants in the confined aquifer after 10,000 years (µg/L). Averaged over the 5 deepest compartments in this aquifer, immediately above the UCG cavity.

Contaminant	AS3-3	AS3-20	AS3-21	AS3-22	AS3-23	AS3-24
		Key Differences From AS3-3				
		Horizontal head gradient higher	Horizontal head gradient lower	No sorption in coal	No sorption As and Zn in aquifers	No sorption As and Zn in aquicludes
Phenol	3E+02	3E+02	3E+02	3E+02	3E+02	3E+02
As	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	7E-06
Zn	<1E-10	<1E-10	<1E-10	<1E-10	<1E-10	3E-05

The greatest increase in concentrations is seen when sorption is disregarded in the aquicludes (see Figure 10 for the evolution of the calculated concentrations of As and Zn in the confined aquifer for these cases). Although As and Zn concentrations are still increasing after 10,000 years, it should be noted that assuming no sorption in aquicludes is very conservative. Hence, it is unlikely that such situation would occur and it if does, the results show that the calculated values are below EQS.

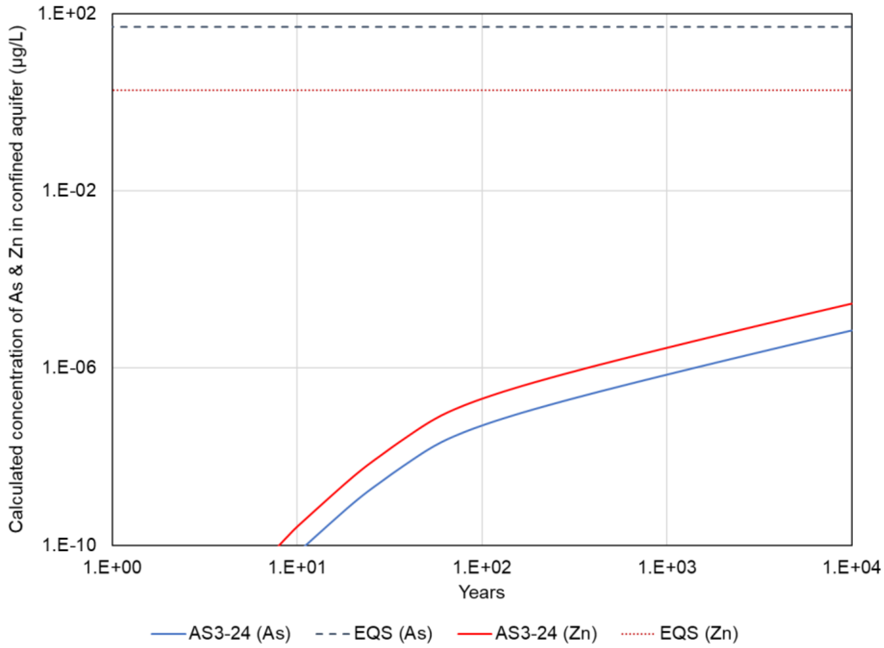

Figure 10. Calculated concentration of As and Zn in the confined aquifer for the AS3-24 case (µg/L).

4.5 Conductive Fault (AS4)

An advective feature, with an aperture of 0.01m, and a length such that it extends the full width or length of the UCG system is assumed to be present just outside of the system. As with the well failure scenario, it is assumed that the fault is downstream of the UCG system with respect to the groundwater flow direction. Hence, this scenario considers the presence of a conductive fault with (AS4-1 and AS4-5) and without (AS4-2, AS4-3, AS4-4 and AS4-6) a 100 m of roof collapse. Further, cases AS4-5 and AS4-6 consider the presence of an upward vertical hydraulic gradient.

Contaminant fluxes in the fault depend on contaminant concentrations at the intersection of the fault with the coal seam that contains the UCG cavity, the fault's transport properties and the hydraulic gradient along the fault. The contaminant concentrations at this fault-coal seam intersection are lower than the contaminant concentrations in the cavity, by an amount that depends on the degree of contaminant attenuation within the coal seam. Contaminant concentrations in the water within the coal seam decrease with increasing distance from the UCG cavity. It follows that for a given set of fault properties and a given hydraulic gradient, the fluxes of contaminants in the fault will also decrease as the distance of the fault from the cavity increases.

In the example model presented here, the fault is positioned 100 m downstream of the UCG cavity. This is pessimistic because a UCG project would likely be sited to be more remote from large conductive faults. Owing to the attenuation between the UCG cavity and the fault, the concentrations of the contaminants are considerably lowered compared to the contaminants in the cavity.

In the absence of any upwards vertical hydraulic gradient, the calculated concentrations of contaminants in the confined aquifer are extremely small (less than 10E-10 µg/L).

5 Conclusions

This paper presented a risk assessment methodology for UCG technology, based on an established methodology for radioactive waste repositories. The assessment methodology can be applied at any stage in a project, between initial planning and final site abandonment.

Central to the approach is the analysis of scenarios which describes the evolution of a system consistent with an assumed set of starting conditions and subsequent events and/or processes that affect the system. The key features, events and processes (FEPs), based on international literature, have been used to describe the behaviour of UCG system in respect of the long-term safety and its performance following the termination of gasification.

In the methodology that has been developed for assessing post-abandonment environmental risks from UCG, each scenario represents a "source-pathway-receptor" combination and its evolution. Here, a Reference Scenario (RS) describing the expected performance of the system and its evolution with time, and several lower probability Alternative Scenarios (AS) exploring deviations from the expected evolution have been developed and analysed using a numerical model. The datasets have been adopted from the literature and do not represent a particular target UCG site. Their use primarily enables illustrations of the risk assessment methodology of a hypothetical UCG project.

Results of the RS suggest that contaminant concentrations at evaluation point are far below any level that could reasonably be detected. In some AS, the calculated concentrations showed an increasing trend at the end of the assessment period, potentially approaching levels that conceivably could be detected. However, as such cases are unexpected and pessimistic, their inclusion is to indicate worst cases that could happen, rather than to give prediction. Alternatively in such situations, the assessment time could be expanded to calculate the peak contaminant concentrations and demonstrate the decreasing trend.

Overall, this illustrative application does demonstrate that plausibly the risks of groundwater contamination from a UCG site considered should be very low if the site is developed and operated appropriately. The outcomes from applying the numerical model are intended to demonstrate how the methodology and the numerical model can be readily adapted to different sites, irrespective of their location or depth of targeted coal seams.

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