GEOLOGICAL DISPOSAL OF RADIOACTIVE WASTE
- EFFECTS OF REPOSITORY DESIGN AND LOCATION ON POST-CLOSURE FLOWS AND GAS MIGRATION

A thesis submitted to the University of Manchester for the degree of Engineering Doctorate in the Faculty of Engineering and Physical Sciences

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Abstract

Geological disposal is the preferred option for the long term management of British intermediate level radioactive waste. The disposal site is currently being identified, with possible geological environments including fractured crystalline rocks and low permeability rocks such as clay. The selection of the host rock will have an impact on the design of the waste repository. This thesis investigates the ways the behaviour of repository borne gas can be affected by the repository design and the selection of the host rock. Commercially available TOUGH2 package is used to model the resaturation of the disposal facility, along with gas migration out of the repository and towards the ground surface in a generic geology.

A facility located in fractured rock is estimated to resaturate within 6.5 years of its closure. The resaturation time is found to be strongly dependent on the presence and properties of a low permeability liner around the disposal vaults. The inflowing water starts gas generation processes within the repository; gas initially accumulates within the facility, but it is estimated to find its way into the host rock approximately 450 years after the facility has been closed. A maximum outflow rate is reached after approximately 1,000 years. The flow of gas migrating through the host rock is strongly affected by site-specific features. In the case of a uniform crystalline rock, gas is found to break through at the surface after 29,000 years.

For a disposal site with a very slow groundwater flow rate, the resaturation phase may take several decades and gas outflow will occur much later. It is estimated that, in very low permeability environments, gas breakthrough may not occur before 100,000 years.
Declaration

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## Glossary

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<td>C-14</td>
<td>A radioactive isotope of carbon.</td>
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<tr>
<td>CH(_4)</td>
<td>Methane.</td>
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<td>CoRWM</td>
<td>Committee on Radioactive Waste Management - An independent body set up by UK Government in 2003 to recommend the best option, or combination of options, for the long-term management of the UK’s higher activity radioactive waste.</td>
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<tr>
<td>Defra</td>
<td>UK Department for Environment, Food and Rural Affairs.</td>
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<td>EBS</td>
<td>Engineered Barrier System. Engineered barriers in the repository aim to limit radionuclide release through the use of physical and chemical barriers.</td>
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<td>EDZ</td>
<td>Excavation Damaged/Disturbed Zone. The zone around the excavation in which the hydrogeological properties of the rock have changed due to changes in the stress state.</td>
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<td>EngD</td>
<td>Engineering Doctorate.</td>
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<td>EOS</td>
<td>Equation-of-State module used in TOUGH2.</td>
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<td>H-2</td>
<td>Hydrogen.</td>
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<td>Definition</td>
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<td>H-3</td>
<td>Tritium.</td>
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<td>HLW</td>
<td>High Level Waste - Radioactive waste which exceeds the upper activity limit for LLW and in which temperature may rise significantly as a result of radioactivity.</td>
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<tr>
<td>ILW</td>
<td>Intermediate Level Waste - Radioactive waste exceeding the upper activity boundaries for LLW but which does not need heat to be taken into account in the design of storage or disposal facilities.</td>
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<tr>
<td>L/ILW</td>
<td>Low and Intermediate Level Waste.</td>
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<td>LLW</td>
<td>Low Level Waste - Radioactive waste having a radioactive content not exceeding 4 gigabecquerels per tonne (GBq/te) of alpha or 12 GBq/te of beta/gamma activity.</td>
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<tr>
<td>MATLAB</td>
<td>MATLAB - MATrix LABoratory - a numerical computing environment which allows easy matrix manipulation and plotting of data.</td>
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<td>MINC</td>
<td>Multiple INteracting Continua - A way of modelling fracture flow in TOUGH2.</td>
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<td>Multi-barrier system</td>
<td>A way of containing radionuclides in a nuclear waste repository through the use of several ‘layers’ of protection, such as physical and chemical barriers.</td>
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<td>MULKOM</td>
<td>Modular structure of TOUGH2 which allows the separation of flow and transport aspects of a problem.</td>
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<td>Full Form</td>
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<tr>
<td>NDA</td>
<td>Nuclear Decommissioning Authority - A non-departmental public body set up in 2005 with designated responsibility for managing the liabilities at specific nuclear sites.</td>
</tr>
<tr>
<td>NEA</td>
<td>The Nuclear Energy Agency - The NEA is a specialised agency within the OECD which assists its member countries in maintaining and developing nuclear energy for peaceful purposes.</td>
</tr>
<tr>
<td>Nirex</td>
<td>Nuclear Industry Radioactive Waste Executive - An organisation previously responsible for developing safe, environmentally sound and publicly acceptable options for the long-term management of radioactive materials in the UK. Nirex operations are now performed by the NDA RWMD.</td>
</tr>
<tr>
<td>NR VB</td>
<td>Nirex Reference Vault Backfill.</td>
</tr>
<tr>
<td>OECD</td>
<td>Organisation for Economic Co-operation and Development. An international body which promotes policies designed to improve the economic and social well-being of people around the world.</td>
</tr>
<tr>
<td>Petrasim</td>
<td>A pre- and post-processor for TOUGH2.</td>
</tr>
<tr>
<td>PGRC</td>
<td>Phased Geological Repository Concept is the proposed disposal concept for the UK ILW and the part of the LLW which is unsuitable for near-surface disposal.</td>
</tr>
<tr>
<td>RE</td>
<td>Research Engineer.</td>
</tr>
<tr>
<td>RWMD</td>
<td>Radioactive Waste Management Directorate. A part of the NDA responsible for disposing of the UK higher activity radioactive waste and thus the programme that delivers the geological disposal facility.</td>
</tr>
<tr>
<td>SILW</td>
<td>Shielded Intermediate Level Waste.</td>
</tr>
</tbody>
</table>
**SWCC**  Soil Water Characteristic Curve is a function, derived from experimental data, which expresses the relationship between capillary pressure and saturation. It is used to predict the simultaneous flow of two fluids.

**SYNROC**  SYNthetic ROCk - ceramic material in which radioactive waste can be immobilised. Used as an alternative for cementitious grouts and bitumen.

**TOUGH2**  TOUGH2 is a program for modelling multiphase, multicomponent fluid flows in fractured and porous media. Other TOUGH family codes include TOUGHREACT and TOUGH+.

**UILW**  Unshielded Intermediate Level Waste.

**WIPP**  The Waste Isolation Pilot Plant. Deep disposal facility for transuranic radioactive waste in the US.
# Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Area ($m^2$)</td>
</tr>
<tr>
<td>$a_L$</td>
<td>Longitudinal dynamic dispersivity ($m$)</td>
</tr>
<tr>
<td>$a_T$</td>
<td>Transverse dynamic dispersivity ($m$)</td>
</tr>
<tr>
<td>$C$</td>
<td>Concentration ($mol/m^3$ or $kg/m^3$)</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion coefficient ($m^2/s$)</td>
</tr>
<tr>
<td>$D_L$</td>
<td>Coefficient of longitudinal hydrodynamic dispersion ($m^2/s$)</td>
</tr>
<tr>
<td>$D_T$</td>
<td>Coefficient of transverse hydrodynamic dispersion ($m^2/s$)</td>
</tr>
<tr>
<td>$D^*$</td>
<td>Effective diffusion coefficient ($m^2/s$)</td>
</tr>
<tr>
<td>$d$</td>
<td>Molecular diffusion coefficient ($m^2/s$)</td>
</tr>
<tr>
<td>$e$</td>
<td>Width of a fault ($m$)</td>
</tr>
<tr>
<td>$F$</td>
<td>Mass or heat flux ($mol/(m^2\cdot s)$ or $kg/(m^2\cdot s)$)</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration ($m/s^2$)</td>
</tr>
<tr>
<td>$H_L$</td>
<td>Henry’s law constant ($kg/(m^3 \cdot atm)$)</td>
</tr>
<tr>
<td>$dh/dl$</td>
<td>Hydraulic gradient ($m/m$)</td>
</tr>
</tbody>
</table>
$K$ Hydraulic conductivity (m/s)

$k$ Intrinsic permeability (m$^2$)

$k_r$ Relative permeability (-)

$M$ Mass or energy per volume (kg/m$^3$ or J/m$^3$)

$m$ Mass (kg), or fitting parameter used in SWCC (-)

$n$ Fitting parameter used in SWCC (-)

$P$ Pressure (Pa)

$P_0$ Gas entry pressure (Pa)

$p_c$ Capillary pressure (Pa)

$Q_{TOT}$ Mass flow rate of fluid (kg/s)

$Q_w$ Fluid discharge (m$^3$/s)

$q$ Specific discharge (m/s), or sink/source in a mass balance equation (kg/s)

$S$ Saturation (-)

$T$ Transmissibility (m$^2$/s)

$V$ Volume (m$^3$)

$v$ Velocity (m/s)

$w$ Empirical coefficient used to calculate effective diffusion coefficient (-)

$X$ Mass fraction (-)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>Fitting parameter used in SWCC (Pa⁻¹), or type of radiation</td>
</tr>
<tr>
<td>β</td>
<td>Type of radiation</td>
</tr>
<tr>
<td>γ</td>
<td>Boundary surface, or type of radiation</td>
</tr>
<tr>
<td>κ</td>
<td>Mass or heat component</td>
</tr>
<tr>
<td>λ</td>
<td>Shape parameter used to define relative permeability and capillary pressure curves (−)</td>
</tr>
<tr>
<td>μ</td>
<td>Dynamic viscosity (Pa · s)</td>
</tr>
<tr>
<td>ρ</td>
<td>Density (kg/m³)</td>
</tr>
<tr>
<td>τ</td>
<td>Tortuosity (−)</td>
</tr>
<tr>
<td>φ</td>
<td>Porosity (−)</td>
</tr>
<tr>
<td>ψ</td>
<td>Air entry pressure (Pa)</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

It is envisaged that the British intermediate level radioactive waste will be disposed of in deep underground facilities. After the repository has been closed, radioactive waste will produce large quantities of gas. This Engineering Doctorate (EngD) studies the behaviour of repository gases in the pressurised environment, and their migration out of the repository and through the host rock. The research aims to provide recommendations to improve the repository design with regards to gas management.

This introductory chapter explains why gas migration modelling is considered as an important aspect of the preparation for radioactive waste disposal. The chapter discusses the concept of an EngD, and the motivation of the sponsoring company and research engineer to engage in it. It also considers the gaps in the current state of knowledge regarding gas migration from radioactive waste repositories, and explains how the EngD project aims to fill some of these gaps. A discussion of what the project hopes to achieve, and how, then follows.

1.1 UK nuclear waste: issues with gas

It has been decided that the UK low and intermediate level radioactive waste will be disposed of in deep underground facilities (CoRWM, 2006; Defra, 2006). Up to the late 1990s, research concentrated on a repository in fractured crystalline rock, which was identified as a potential disposal environment. Extensive experimental and numerical studies to prove the safety of the disposal of radioactive waste in the vicinity of Sellafield took place. However, plans for constructing an underground research facility fell through following a rejection of the planning application in 1997. Almost 10 years later, disposal of radioactive waste deep underground was again deemed feasible. This
1.2. **WHY UNDERTAKE AN ENGINEERING DOCTORATE?**

An Engineering Doctorate involves carrying out a PhD style project, as well as undertaking several management and project specific technical modules and professional development courses. The total duration of the programme is four years.

The sponsoring company, Ove Arup & Partners Ltd (ARUP), has an extensive track record in radioactive waste disposal dating back to the 1980s. In 2005, ARUP tendered to be one of the Nuclear Decommissioning Authority’s (NDA’s) five year design framework contractors on the development of the Geological Disposal Facility. Their bid was, however, unsuccessful. This led to the need to enhance ARUP’s understanding of the technical issues specific to nuclear waste disposal, and thus the establishment of three ARUP-sponsored research projects.

This research project aims to provide ARUP with skills in post closure safety assessment of radioactive waste disposal and, in particular, to enhance ARUP’s in-house knowledge of the modelling practices currently used in the industry. The project also provides opportunities for networking and establishing contacts within the industry. Simon Norris of the NDA is a member of the steering group for the project. This provides ARUP with access to the nuclear decommissioning client body and enables the research to be focussed in a direction that the NDA considers relevant.

The Research Engineer (RE), Elina Kuitunen, became interested in the project after
having completed a bachelors degree in Physics with Business and Management and
a master’s degree in Nuclear Science and Technology at the University of Manchester.
Her MSc studies concentrated on the radioactive waste management practices and the
environmental effect of nuclear power. As part of the degree, she carried out a three-
month placement at Fortum Nuclear Services, Finland. There she investigated the fate
of carbon-14 in near surface disposal facilities. Carbon-14 was found to escape from
the disposal facilities in both gaseous and liquid forms. Whilst the gas route was not
thought to result in radiological hazards, a lot of attention was paid to the migration
of contaminated water from the facility.

At the start of the EngD project, the RE realised that gas migration was considered
to have much more importance in the UK than it did in Finland, which attracted her
attention. A review of the NDA’s outstanding research objectives published in 2005
also showed that the topic was listed as an area requiring further research. Addition-
ally, this was an area where ARUP had existing geological and hydrogeological skills.
The project was thus decided to consider the migration of gases from the Geological
Disposal Facility using numerical modelling.

The success of ARUP’s investment into the research and skills development within the
nuclear field was demonstrated in 2010, when ARUP re-tendered for the framework
contract with the NDA’s Radioactive Waste Management Directorate (RWMD) on
engineering design of the geological disposal facility and transport and waste package
design. The bid was made together with two of ARUP’s partners, Costain and Pöyry.
Together the three companies form the CAP Alliance. The CAP Alliance were chosen
as one of three contractors to carry out this work over a period of 5 years. The con-
tract is estimated to produce an income of up to one million pounds per year. ARUP
also hopes for the CAP Alliance, with its strong geotechnical capabilities, to become
involved in further stages of the geological disposal project, such as the surface inves-
tigations on the potential disposal sites. Implementing geological disposal is expected
to cost the NDA RWMD several billion pounds, and ARUP consider their involvement
in this process as an important long-term goal.

1.3 Project aims and objectives

The Nuclear Energy Agency (NEA/OECD, 2001) recommends that the impacts of gas
should be taken into account in the repository design. This EngD project aims to
identify features which affect gas generation, containment and migration from deep
1.4 Scope and specification

The project involves modelling gas migration in different environments which have been identified as being suitable for the UK deep geological disposal facility. The work addresses repository location, design and layout issues through a parametric study. The project does not aim to provide detailed 3D models of the repository, and/or a specific disposal site, as this work is being carried out by the NDA. Instead, generic features in both near and far fields are considered. The project scope is further discussed in Chapter 4.

1.5 Contribution to science

Gas migration modelling performed to date falls mainly under two categories: either the modelling is limited to very simple cases, or a detailed repository design has already been prepared for a specific disposal site and the aim of the modelling is to demonstrate that gas migration does not pose a threat to the design. Metcalfe et al. (2008) argue that gas migration in the geosphere depends on site-specific features to such a large extent that the number of modelling activities should be limited until the repository location is decided upon.

This research will, therefore, use the properties of generic disposal sites and repository designs, and provide a study of their effects on gas migration. In particular, this piece
of research will address the following issues which have not previously been considered:

- The research will study the effects of different repository features on fluid flows within the repository and around it, comparing their relative importance.

- The behaviour of gases in different, non-homogeneous, host rocks without using a specific disposal site will be evaluated.

The project will provide a proactive approach to gas management, rather than attempting to demonstrate the safety of existing repository designs. It is hoped that this information can be used to select the repository location and design to be such that gases can be managed effectively.

### 1.6 Thesis outline

This chapter gave a broad overview of the EngD research and how it ties in with the sponsoring company ARUP’s long term goals. A brief introduction to the EngD programme was given, and the benefits of the research to both ARUP and the wider scientific community were discussed. The aims and objectives of the research were also outlined.

The disposal of radioactive waste in the UK is considered in more detail in Chapter 2. The chapter explains why it was decided to dispose of intermediate level radioactive waste in an underground repository, and why gas production is considered to be a problem. It also discusses techniques to manage repository gases.

Chapter 3 considers the mathematical representation of two-phase fluid flow in porous media. First, concepts essential to understanding behaviour of gases and two-phase flow are introduced. Laws governing advective flow and hydrodynamic dispersion are then presented. Particular attention is paid to the ways of representing relative permeability in fluid flow calculations.

Chapter 4 discusses the scope of the EngD project in more detail. Numerical gas migration studies carried out to date are then summarised. Finally, TOUGH2, software commonly used in the nuclear industry for gas migration studies, is introduced.

The behaviour of repository gases in the pressurised two-phase environment is demonstrated in Chapter 5 with the aid of simple TOUGH2 calculations. These examples
show how gas compresses and dissolves in the repository, and how rock features affect the migration of gases through the host rock.

Chapter 6 builds on the modelling presented in the previous chapter and considers the resaturation process of the repository. Detailed 3D models of the repository vaults and tunnels are used to estimate the time it takes for the repository to fill with water. The effect of the repository design and layout on the resaturation time is evaluated through a parametric study.

Chapter 7 considers the behaviour of gases within the repository. The rate at which gas escapes from the repository is calculated, taking into account the location of the repository and the choice of different materials within the disposal units.

Studies of the migration of gas through the geological medium is then presented in Chapter 8. These calculations evaluate the impact of host rock features, such as low permeability caprocks and high permeability faults, on the gas migration.

The concluding chapter presents the conclusions drawn from the resaturation and gas migration studies and provides recommendations regarding the repository design. Scope for future work is also discussed.

The appendices at the end of the thesis provide additional information regarding the project. Appendix A provides an internal memorandum prepared by an ARUP employee, Steve Macklin, on parameter choices. Appendices B, C and D contain copies of conference and journal articles published as part of the project.
Chapter 2

L/ILW Disposal in the UK

The UK radioactive waste is divided into three categories: Low Level Waste (LLW), Intermediate Level Waste (ILW) and High Level Waste (HLW). This project considers the long term disposal options for ILW and some LLW which is considered unsuitable for near-surface disposal. Together these wastes are referred to as low and intermediate level radioactive waste (L/ILW). This chapter discusses the current plans to dispose of L/ILW in a geological disposal facility. The chapter presents the quantities of waste requiring deep disposal and the development of the UK repository concept. The proposed repository design is introduced and its main components discussed in detail.

The types of radioactive waste produced in the UK are expected to produce large quantities of gas. Most of the gas will be produced as a result of corrosion of waste packages and repository structures, and will thus be non-radioactive. However, as the gas forms a pathway out of the repository, some radioactive gas may also escape. The chapter explains which radionuclides need to be considered in safety assessments considering gas migration, the types of gases they may become incorporated into, and how these gases are formed. The repository barrier system is designed to prevent radionuclides from leaving the disposal facility. The chapter considers the different components of the barrier system, including both engineered and natural features, affecting gas migration.

2.1 Waste inventory

LLW is radioactive waste which has a radioactive content of less than 4 GBq/te of alpha or 12 GBq/te of beta/gamma activity. LLW includes reflector and shield graphite from reactor cores, organic materials and decommissioning wastes such as soil, building rubble and steel items. Most of UK LLW is disposed of in the Low Level Waste Repository near Drigg in Cumbria. The LLW considered in this project consists of low
level waste unsuitable for near-surface disposal at the LLW Repository, often due to its high concentrations of carbon-14.

ILW is radioactive waste which exceeds the activity limit for LLW but which does not produce heat. Heat producing HLW and spent nuclear fuel are not considered in this project. ILW arises mainly from the reprocessing of spent nuclear fuel, and from general operation, maintenance and decommissioning of nuclear facilities. The majority of ILW consists of metal items such as fuel cladding and reactor components, organic materials, graphite from reactor cores and sludges from the treatment of liquid effluents. ILW also includes building materials such as cement, rubble, soil, glass and ceramics. For disposal purposes, ILW is divided into two categories according to its packaging: shielded (SILW) and unshielded (UILW). UILW requires additional radiation shielding to be used during handling and transport of the waste.

The current estimated total volume of waste for geological disposal (NDA, 2010c) is shown in Table 2.1. This estimate is based on the waste inventory by Defra (2008). The figures take into account the operation and dismantling of existing nuclear power stations, but ignore the waste arising from the new-build programme.

<table>
<thead>
<tr>
<th>Waste type</th>
<th>Packaged volume</th>
<th>Number of packages</th>
</tr>
</thead>
<tbody>
<tr>
<td>ILW</td>
<td>364,000 m$^3$</td>
<td>200,000</td>
</tr>
<tr>
<td>LLW</td>
<td>17,000 m$^3$</td>
<td>approximately 400</td>
</tr>
</tbody>
</table>

Table 2.1: Waste volume estimate (based on NDA, 2010c; Defra, 2008).

Approximately 1% of the total volume of current and estimated future arisings of radioactive waste is produced as a result of defence activities (Defra, 2010). This waste remains under the ownership of the Ministry of Defence and is not considered further in this thesis.

There is considerable uncertainty in the estimation of the total volume of waste. The activity concentrations of certain types of wastes are not fully known, and the future arisings of waste depend on, for example, the life time of the reactors and the classification of waste. The NDA (2010c) have estimated an upper inventory of ILW to be approximately 60% higher than the baseline inventory considered in Table 2.1.
CHAPTER 2. L/ILW DISPOSAL IN THE UK

2.2 L/ILW disposal programme

There is currently no long term disposal route for radioactive waste which is considered unsuitable for near-surface disposal. Efforts to find a solution to this problem began with a report presented to the Government in 1976 (Flowers, 1976). The report indicated the need to establish an independent advisory body responsible for developing nuclear waste disposal policies. As a result, the Nuclear Industry Radioactive Waste Executive (Nirex) was formed in 1982. Nirex was made responsible for dealing with the UK solid L/ILW. The Government then announced plans to dispose of ILW, together with the part of the LLW which is unsuitable for near-surface disposal, in a deep geological repository.

Nirex began large-scale investigations into the geological disposal of L/ILW. The R&D programme carried out in the 1980s resulted in the development of the Phased Geological Repository Concept (PGRC), which is now the reference UK disposal concept (Hicks et al., 2008). It identifies steel or cement containers emplaced in underground caverns, surrounded with a cementitious backfill material, as the preferred method for waste disposal. The PGRC employs a multi-barrier approach designed to prevent radionuclides from migrating out of the repository.

In 1991, Nirex concentrated their site investigations at Sellafield, and carried out extensive investigations into the suitability of the site for geological waste disposal. However, the planning application for an underground research facility was rejected in 1997, and the UK geological disposal programme was completely halted. Two years later, the disposal of radioactive waste in a deep repository using the PGRC was again deemed feasible. The Nuclear Decommissioning Authority (NDA) was set up in 2005 and made responsible for the decommissioning and clean up of the UK’s civil nuclear legacy. The following year, the Committee on Radioactive Waste Management (CoRWM) recommended a partnership approach between the Government and potential host communities for the disposal facility (CoRWM, 2006). This brings us to the present. Volunteer communities are currently being identified, and this phase will be followed by in-depth site investigations to determine the suitability of each site. The number of disposal sites is currently unlimited, which may result in several facilities being built at different locations.
2.2. L/ILW DISPOSAL PROGRAMME

2.2.1 Repository Design

The PGRC introduces disposal plans for L/ILW in a deep underground repository. It assumes a repository excavated at a depth of 300 m - 1000 m, but does not specify the location or the type of host rock. The possible host rocks include high strength crystalline rocks, which only require limited support, and sedimentary and evaporite rocks such as limestone, mudstone, sandstone, clays and salt, where considerable support for underground structures would be required. A reference case design in a low permeability high strength crystalline rock has been developed the furthest, but other environments are still possible.

The repository will initially be used as a research laboratory until the suitability of the rock is confirmed. Planning consent will also need to be obtained before the repository construction can start. After construction, the facility will be used as a store for radioactive waste until a decision is made by future generations to close the facility.

The general features of the geological disposal facility are shown in Figure 2.1. Several options for the repository design were considered. These included the use of vaults, tunnels, silos, boreholes and shafts, and options of locating the repository under land or under the seabed (Hicks et al., 2008). Vaults are the largest spaces that can be constructed in any particular rock stratum. Waste emplacement and backfilling would be performed using equipment at the top of the vaults. Tunnels are distinguished from vaults by the way they are used: no access for personnel or equipment would be available on the top or sides of waste packages, and waste emplacement and backfilling would be conducted from the same direction. Low lift heights would reduce the severity of drop accidents in both cases. After initial consideration, vaults were chosen as the preferred option for hard rock sites due to the maximum packing efficiency and thus reduced cost. Tunnels were recommended for softer sedimentary formations where more support would be needed than in hard rock environments. It is also recognised that it is possible to use smaller vaults and silos if appropriate for the disposal site. Silos are vertical cylindrical underground openings that require less rock support than vaults. Emplacement in a silo would, however, require waste packages to be lowered through a large distance, which may prove problematic.

A vault is a long rectangular opening that can be constructed to a depth of 1000 m in strong sedimentary rocks. At depths greater than 500 m, the vault shape may change from a rectangle to ‘D’ or horseshoe shape. The vaults are currently expected to be approximately 300 m long, 16 m high and 16 m wide (Nirex, 2003b). In weak sedimentary rocks, circular cross sections would be preferred and high levels of support needed. The
CHAPTER 2. L/ILW DISPOSAL IN THE UK

Figure 2.1: General features of the geological disposal facility (image taken from NDA, 2010a).

Repository would be excavated at a depth of 300 m - 500 m. Tunnels with diameters of 6 m - 8 m, or small vaults with diameters of approximately 6 m, or larger D-shaped vaults, could be constructed. Repository dimensions in evaporite rocks are difficult to predict without site specific information and vault heights would be constrained by the deposit thickness.

According to the most recent design (NDA, 2010a), access to the reference case repository is provided by three access routes: a drift which is 4 km long and has a diameter of 5.5 m, and two shafts with diameters of 8 m and 5 m. The drift is equipped with a rack-railway locomotive system which would be used for the transfer of packages underground and the return of empty transport containers to the surface. Waste canisters will be placed in vaults or tunnels, as opposed to in-floor disposal preferred by many other countries, in order to maximise disposal volume.
Figure 2.2: The Phased Geological Disposal Concept (image taken from NDA, 2010a).
2.2.2 Phased operations

The PGRC involves the disposal of radioactive waste to be carried out in phases, as shown in Figure 2.2. The first phase is normally carried out at the site of waste production, where the waste is immobilised in cement and packaged in steel or concrete containers. The waste packages then undergo a period of interim storage before transportation to the final disposal facility. At the disposal site, the packages are emplaced in the underground vaults or tunnels.

The waste emplacement phase is expected to last approximately 90 years, during which the construction of the facility will be finished in parallel. This may then be followed by a care and maintenance phase lasting up to a few hundred years. During this phase, temperature, pressure, moisture, and chemical conditions of the facility would be controlled in order to maintain the wastes in favourable conditions.

The backfilling of the repository will be carried out when it is deemed necessary by future generations. This so-called ‘deferred backfilling’ is currently the preferred option instead of immediate or staged backfilling. This allows the use of most recent knowledge in the backfilling operations, and the retrieval of wastes for up to several hundred years. Problems with deferred backfilling, however, include the need to build in backfilling equipment during repository construction, which means leaving the equipment to deteriorate in the repository conditions until the operations are started. The backfilling phase is followed by the sealing and closure of the repository. After this only non-intrusive techniques will be used to monitor the wastes.

2.2.3 Repository conditions after closure

During the operational phase of the repository, groundwater and gases will be removed by pumping and the repository is kept at atmospheric pressure. Immediately after repository closure, there is a large pressure gradient between the facility and the surrounding fully saturated host rock. This may lead to a high initial rate of groundwater flow into the repository. As the groundwater gradually fills all void space within the repository, such as pore space within the backfill and the crown space, the repository conditions change: The conditions will become highly alkaline due to the dissolution of alkali metal hydroxides from the backfill (Nirex, 2003a). In addition, aerobic corrosion will consume oxygen and the conditions will eventually become reducing.

The temperature of the repository may reach 80 °C during backfilling stages (Nirex,
2.3. REPOSITORY GASES

2003b), but will then reduce to values around 35 – 50°C. The long term maximum temperature target set by the NDA is 50°C. After several hundred years, the conditions in the repository will be anaerobic, reducing and highly alkaline. The wastes will have resaturated and the integrity of the waste containers starts to decline due to corrosion. After around 100,000 years, the waste containers are likely to be completely degraded and they no longer form a barrier to flow. The repository pH will slowly reduce and the temperature will be close to ambient conditions.

2.3 Repository gases

Radioactive wastes placed in the repository can degrade by several mechanisms giving rise to gas generation; large quantities of gas are expected to be formed. These gases may accumulate within the repository and cause increased pressures. Alternatively, they may migrate to the ground surface and result in radiological exposures. Although the bulk of the gas is expected to be non-radioactive hydrogen, some radioactive gases may also form. It is therefore important to investigate and evaluate the gas generation processes, and the migration of gases in the geosphere, in order to estimate their possible consequences. This section introduces the radionuclides present in the radioactive waste and the mechanisms by which they may become incorporated into gaseous forms.

2.3.1 Radionuclides present in the repository

Due to the long time scales associated with radioactive waste disposal, some radioactive material is expected to be released from the facility. The radionuclides that are thought to be capable of causing radiological exposures are introduced below.

Tritium

Tritium (H-3) is widely distributed in radioactive wastes. It has a relatively short half-life of 12.35 years, and the tritium inventory in the repository is thus likely to decay to insignificant levels in a few hundred years. If tritium is transported away from the repository with the groundwater, it is unlikely to cause radiological exposures to the general public (Thorne, 2005b). Tritium can, however, be incorporated into several different gaseous species, including hydrogen and methane (CH₄). These gases are expected to be unreactive in the geosphere and can migrate to the ground surface rapidly if a gas pathway becomes established. Due to this reason, and the fact that
there are substantial amounts of tritium available in the repository, it is necessary to consider it as one of the radionuclides capable of causing radiological exposures.

**Carbon-14**

Carbon-14 (C-14) has a half-life of 5,730 years. C-14 is created in reactor metals primarily as a result of neutron capture by nitrogen atoms through $^{14}\text{N}(n,p)^{14}\text{C}$ reaction during operation. C-14 is also present in graphite and organic wastes. C-14 atoms can be incorporated into several different chemical forms, both inorganic and organic. While the retardation mechanisms of inorganic compounds, such as carbon dioxide, are rather well understood, the ways in which organic compounds migrate out of the repository are less clear. Organic compounds have low solubilities and are expected to be non-reactive in the repository nearfield. The main potential hazard from C-14 bearing gases, in terms of radiological dose, is thus considered to arise from organic species.

Inorganic compounds considered here consist mainly of C-14 labelled carbon dioxide. The geochemical behaviour of carbon dioxide is strongly affected by the alkaline repository environment, in which C-14 labelled $\text{CO}_2$ transforms into inorganic calcium carbonate through a carbonation process. The release of C-14 is then mainly controlled by the solubility and dissolution kinetics of calcium carbonate. The solubility of calcium carbonate in a solution saturated with portlandite is very low, and examples from the natural environment have been used to show that a C-14 release from the repository would be very unlikely (Dayal and Reardon, 1992). It is however possible that the repository conditions are very different from those of the naturally occurring $\text{CO}_2$ storages and the repository $\text{CO}_2$ may be able to escape. It may also be possible for $\text{CO}_2$ to react with hydrogen to produce methane.

The main organic radioactive gas to be generated in the repository is expected to be carbon-14 labelled methane. Methane has a low solubility and is likely to be non-reactive in the repository and the geosphere. It can therefore be transported to the ground surface more easily than carbon dioxide. Other possible organic gases include for example acetylene, ethylene and ethane, which also migrate through the geosphere easily (Thorne and Mackenzie, 2005).

**Radon-222**

The long-lived radionuclide radium-226, present in some waste streams, produces a continuous supply of radon-222 as it decays. Radon is the only significant gas produced by
2.3. REPOSITORY GASES

radioactive decay in ILW packages. The isotope $^{222}\text{Rn}$ has the longest half-life of 3.82
days but this is sufficiently short, in comparison with other radionuclides, for much of
the gas not to escape from the waste container. As radon-222 is a noble gas, it is not
expected to react with the waste package or its contents and it will migrate away from
its site of production by diffusive processes.

2.3.2 Gas generation processes

After the repository is closed, gas generation processes are expected to produce large
quantities of gas. Most of the gas will be non-radioactive, but radionuclides present
in the repository may react with hydrogen to form radioactive gases such as carbon
dioxide and methane labelled with carbon-14, or methane and hydrogen labelled with
tritium. The main gas generation processes are introduced below.

Metal corrosion

Corrosion reactions are responsible for the generation of the bulk gas, hydrogen. Metals
present in the waste stream include for example magnox (an alloy of magnesium used
in nuclear fuel cladding), irradiated uranium, stainless steels, aluminium and zircaloy
(an alloy of zirconium also used in nuclear fuel cladding). The rate of the corrosion
reactions depends on the availability of water and oxygen.

Irradiated metals also often contain radionuclides such as C-14 as a result of neutron
capture by nitrogen atoms, tritium that has diffused into the metal at high temper-
atures, and some noble gas isotopes such as Kr-81, Kr-85, Ar-39 and Ar-42. These
radioactive isotopes can escape as the metal corrodes and thus result in the formation
of radioactive gases. The release of C-14 and tritium can result in the formation of sev-
eral different C-14 and H-3 bearing gases such as carbon dioxide, methane and tritiated
hydrogen. The rate of release of such gases is strongly dependent on the distribution of
these atoms in the metal. Additionally, the molecular form of C-14 in the metal affects
the type of gas that can be formed. If carbon is present as carbides, it is thought that
hydrocarbons such as methane, acetylene, ethylene and ethane can be formed when
the carbides become exposed on the metal surface and contact groundwater (Thorne,
2005a). If elemental carbon is present, the formation of organic gases is unlikely. The
exact form of C-14 atoms in metals is, however, not known (Hicks et al., 2003).
Radiolysis

Radiolysis means the dissociation of molecules by radiation and it may be a significant source of gas released from ILW at early times. Radiolysis of water and aqueous solutions produces hydrogen (Rodwell et al., 2003). If the water contains tritium, then the hydrogen produced will also be tritiated in the corresponding proportion. Water within the waste package can be subjected to radiolysis from $\alpha$, $\beta$ and $\gamma$-radiation. Water external to the package may also be hydrolysed by $\gamma$-radiation escaping from the package, although this is less relevant to L/ILW. Radiolysis of organic compounds present in the wastes produces a variety of gases, of which hydrogen is expected to be the most important. Some organic wastes may contain C-14 which can then be released as a gas.

Microbial degradation of organic wastes

The degradation of cellulose and small soluble organic molecules is considered to produce gases (Thorne, 2005a). Cellulose is initially hydrolysed to small organic molecules which are then degraded to produce CO$_2$ or CH$_4$. Methane is only produced in anaerobic conditions and in the absence of nitrate and sulphate ions (Hoch and Rodwell, 2003); nitrate and sulphate thus play a major role in preventing CH$_4$ production from the organic wastes. Some microbially degradable small molecules may contain C-14 which could be incorporated into gases.

Other gas generation processes

Other gas generation processes in the repository include solid state diffusion and the release of ‘trapped’ radioactive gases from graphite (see for example Rodwell, 2004). Solid state diffusion implies the movement and transport of atoms in solid phases. This includes the release of tritium and some noble gas isotopes ($^{81}$Kr, $^{85}$Kr, $^{39}$Ar, $^{42}$Ar) from metals.

Carbon-14 in graphite is formed through two reactions: irradiation of nitrogen impurities and neutron capture by C-13 atoms present in the metal in small quantities. It is estimated that the inventory of C-14 in solid graphite accounts for about 80% of the total C-14 inventory (Norris and McKinney, 2008), but it is uncertain whether, and at what rate, the C-14 could be released. Some graphite may also contain tritium. The releases of C-14 bearing gases and tritium can occur as the graphite degrades, or by solid-state diffusion. Marsden et al. (2002) suggest that C-14 is likely to be released as carbon dioxide. Other authors note that both organic and inorganic forms may be formed from graphite (see for example Magnusson, 2002) and the releases are likely to
be in the form of carbon dioxide and/or methane.

### 2.3.3 Gas generation rates

The estimated quantities of hydrogen and methane to be formed in a repository are shown in Figure 2.3. The quantity of hydrogen produced is several orders of magnitude larger than that of methane. Hoch and Swift (2010) estimated that a peak production rate of hydrogen of approximately $1 \times 10^6$ m$^3$/yr occurs due to corrosion during the repository resaturation phase, but that the rate falls down to approximately $1 \times 10^3$ m$^3$/yr within 30 years. Additionally, some carbon dioxide may be produced.

![Figure 2.3: Estimated gas generation rates from the UILW in a repository located in fractured rock (image taken from Hoch and Swift, 2010). The release rates of hydrogen and methane are shown as volumes generated per year (vertical scale on the left), while the release rates of tritium, radioactive methane and radon are shown as radioactivity released per year (vertical scale on the right). The horizontal axis shows the time in years AD.](image)

The gas generation rates depend on the waste inventories and materials used in the repository, along with repository conditions. Some of the factors controlling gas generation rates are listed below.
Availability of water

The availability of water affects the corrosion rates of metals, thus having a direct effect on the gas generation rates. Water is also required for microbial reactions; if there is little water available initially, the degradation of organic wastes during operation is restricted. Increased quantities of gas could then be produced after the repository has been closed.

pH

The interaction of groundwater with the cementitious backfill material is expected to cause the pH to rise to approximately 12.5 (Nirex, 2003a). In highly alkaline conditions, the corrosion rates of metals and the solubility of radionuclides are considerably reduced.

Temperature

Temperature affects the rates of corrosion and microbial activity. Temperature may also affect the repository pH and the solubility of repository materials.

Microbial populations

Microbial populations degrade organic material. If only low populations are present at the time of emplacement, more C-14 bearing organic material is left for consumption in the anaerobic rather than aerobic conditions. This means that an increased amount of methane could be generated after the repository closure.

Anaerobicity

In anaerobic conditions, the production of methane prevails. Pockets of anaerobicity may form in the waste packages before repository closure and increase the generation rate of methane during operation. This has implications on the gas generation rates after closure.

Nitrate

The presence of nitrate ions increases the populations of the nitrate-reducing microbes and slows down the growth of microbes involved in methane production. If nitrate levels in the wastes are significantly reduced, the methane production is expected to increase.
2.4 Near field management of gases

Radionuclides may become incorporated into gases or groundwater, and thus migrate out in gaseous or dissolved forms. The repository will be designed so that both natural and engineered features will be used to prevent the radionuclides from escaping. Some disposal concepts rely on the host rock to prevent radionuclide migration into the surrounding environment, whereas others place much more importance to the Engineered Barrier System (EBS).

The UK concept may involve radioactive waste disposal in a fractured rock environment, through which significant groundwater flow may occur. In such an environment, it is the role of the EBS to contain short-lived radionuclides and to limit the long-term release of long-lived radionuclides. This can be done by controlling groundwater transport in and around the repository, by limiting radionuclide solubilities and by providing sorption surfaces for radionuclides. The EBS consists of several possible elements, such as the waste packages, backfill and seals used in the repository. This section discusses the barrier system and different repository features that deal with gases.

2.4.1 Multi-barrier concept

The multi-barrier system is based on the idea that the safety of the repository is not completely reliant on any one barrier, or the actions of future generations. The barrier system consists of both man-made and natural features. NDA (2010a) consider the barriers to be physical containment, chemical conditioning and geological containment.

2.4.1.1 Physical containment

Physical containment involves a steel or concrete container within which the radioactive waste has been immobilised using a cementitious fill material. The main function of the waste package is to contain short-lived radionuclides until they have decayed to insignificant levels. The waste container and immobilised wasteform provide a barrier for groundwater access to the waste, thus limiting the dissolution and transport of radionuclides within the groundwater. The container also enables handling of the waste during storage, transport and emplacement in the repository. Most containers are vented in order to prevent the build-up of internal gases, and some long-lived nuclides are therefore expected to be released with gases escaping from the waste containers.
Figure 2.4 shows the most common waste package, a 500-litre drum, and the cementitious wasteform within it.

Radioactive waste must be converted into passively safe, solid wasteforms which means immobilising liquids, sludges and fragmented solids. Common immobilisation matrices include cement, bitumen, organic polymers, the products of high-temperature incineration and melting, phosphate ceramics, glasses and glass ceramics, SYNROC and natural crystalline mineral phases. The most common immobilisation matrix is cement. Cementitious immobilisation materials condition the chemical environment of the wasteform to high pH values which ensures low solubility of many radionuclides. Wastes immobilised in cements are easy to handle and the immobilisation matrix can be modified to suit different wasteforms: liquid and sludge wastes are mixed with cement within or outside the disposal containers to form a relatively homogeneous wasteform, solid wastes are placed in containers which are then filled with fluid cement grout, and super-compacted wastes are often surrounded by an annulus of concrete grout within disposal containers. Cements have also been considered advantageous due to their low cost, availability and good chemical, physical and thermal stability.

It has been considered unnecessary in the UK to use self-shielding packages for all the radioactive waste, due to the increase in the package size and weight which increase the disposal costs. The focus has instead been given to the development of standard unshielded and shielded containers. Six standard packages have been described: four
unshielded packages (a 3 m\(^3\) box, a 3 m\(^3\) drum, a 500 litre drum and a 4 m box) and two shielded packages for less radioactive wastes which do not require additional shielding during transport and operations (a 2 m box and a 4 m box). Figure 2.5 shows the standard waste packages. Additionally, waste producers are allowed to develop their own containers provided these comply with the same requirements as the standard containers. These containers are intended mainly for use in the hard rock repositories and further development may be needed should a different repository environment be chosen.

Some other physical containment features can also be used to contain radionuclides within the disposal vaults. For example, shotcreting the vault walls with a low-permeability material affects the rate at which groundwater flows into, and contaminated water and gases flow out of, the vault.
2.4.1.2 Chemical conditioning

The second barrier is formed by the repository backfill material. The backfill is likely to consist of a cementitious material which will act as a chemical buffer and create uniform alkaline and chemically reducing conditions in and around the repository. Under alkaline and reducing conditions, the solubilities of many radionuclides will be reduced. Additionally, the high pH environment provided by the cementitious backfill will decrease the corrosion rates of steel containers and thus reduce the release rate of radionuclides. Backfill will also provide a surface for radionuclide sorption due to its relatively high porosity. Additionally, it can be used as mechanical support and as a barrier to minimise groundwater flow around the wastes.

The UK has developed a patented cementitious backfill material called the Nirex Reference Vault Backfill (NRVB) - a mixture of Portland cement, water, hydrated lime and limestone flour (Crossland and Vines, 2001). The NRVB is a porous cement which allows gas migration through it. As a chemical barrier, it will create a high pH environment in the repository and thus limit radionuclide solubilities in the long term. Other options such as no backfill, clay and loose aggregates have also been considered, but the NRVB has been found to have a superior long-term performance and to be physically and chemically compatible with the UK wasteforms. Another commonly used backfill material is bentonite clay which swells on contact with water and thus plugs all openings. Bentonite is expected to ensure diffusion-controlled solute transport, act as a colloid barrier and retard radionuclide transport (Hicks et al., 2008).

2.4.1.3 Geological containment

The final barrier involves the sealing and closing of the repository in a suitable geological environment in order to isolate it from the living environment. The repository will be overlain by several hundred metres of rock, making accidental entering difficult and preventing natural processes, such as erosion, from damaging the containment capability of the repository. The French and Swiss concepts involve disposal in a low permeability clay environment. These concepts consider the ability of the host rock to retard radionuclide migration to be the primary barrier.

A favourable disposal environment would be a low-permeability host rock with little groundwater flow through it. Short-lived radionuclides are expected to decay within the repository, but some long-lived radionuclides are likely to migrate out. The disposal depth should be chosen to be such that, when this occurs, decay, sorption and
dispersion processes limit the concentrations of the radionuclides on the surface. After the repository is backfilled, all the disposal vault entrances and exits will be sealed using low-permeability materials. These contribute to the containment capability of the repository, and prevent access tunnels and shafts from becoming preferential pathways for radionuclide migration.
2.4.2 International disposal concepts

Hicks et al. (2008) divide the different disposal concepts into four categories: disposal of waste in weak rock with little or no groundwater flow, disposal in strong rock with little or no groundwater flow, disposal in strong rock with potentially significant groundwater flow and disposal in plastic evaporite rock with no groundwater flow. These are introduced in Table 2.2.

Some countries employ techniques not proposed in the UK concept, which could be considered in order to provide additional safety features. In the Swiss concept wastes containing nitrates and chelating agents will be isolated from the rest of the wastes. This is done in order to limit their potential to affect the other wastes through increased solubilities or decreased sorption of radionuclides in the presence of these substances. The French divide the disposal zone into two separate areas, with any organic materials being separated from the other types of wastes. The wastes are also conditioned according to their type - some wastes, such as sludges, in bitumen, others in concrete. Some countries, such as Japan, France and Sweden, also use specific package and vault designs for different waste streams.

Sweden and Finland are actively researching the option of placing radioactive waste in a hard rock environment where groundwater flow is significant. In addition to using concrete grout to fill the spaces between the waste packages, crushed rock is used to fill the spaces between vaults and cavern walls. Crushed rock is intended to serve as a hydraulic cage which smooths out and diverts groundwater flow and discourages flow through the concrete barrier.

The Waste Isolation Pilot Plant (WIPP) in the USA is constructed in a low-permeability salt rock horizon. Re-usable casks are used during operation and the wastes are emplaced in pre-drilled holes in the repository room walls. The holes are subsequently plugged. The use of magnesium oxide forms an important part of the concept (Hicks et al., 2008); sacks of MgO are disposed of with the waste. The wastes will be encapsulated in the repository by creep closure of the host rock which will form a low-permeability barrier around the waste packages. The MgO sacks will then break open and consume moisture and CO₂ that could be produced in the repository. It will also buffer the repository pH and limit the solubilities of actinides. In-situ gas sorption has also been considered in the UK. It is known that methane and CO₂ are strongly absorbed by coals (see for example Bate et al., 2007). Anthracite, for example, is capable of sorbing substantial quantities of CH₄ and CO₂ at the hydrostatic pressure at a typical repository depth. It may therefore be possible to retard the migration
### 2.4. Near Field Management of Gases

<table>
<thead>
<tr>
<th>WEAK ROCK</th>
<th>STRONG ROCK</th>
<th>STRONG ROCK</th>
<th>PLASTIC EVAPORITES</th>
</tr>
</thead>
<tbody>
<tr>
<td>(little or no groundwater flow)</td>
<td>(little or no groundwater flow)</td>
<td>(significant groundwater flow)</td>
<td>(no groundwater flow)</td>
</tr>
<tr>
<td><strong>Countries</strong></td>
<td>Belgium, France, Japan, Switzerland</td>
<td>Canada, Japan</td>
<td>Sweden, Finland</td>
</tr>
<tr>
<td><strong>Host rock</strong></td>
<td>Indurated/plastic low permeability sedimentary rock</td>
<td>Crystalline rock</td>
<td>Crystalline rock, carbonate</td>
</tr>
<tr>
<td><strong>Primary barrier</strong></td>
<td>Host rock most important barrier. Self-healing of cracks and fissures an important property of the rock.</td>
<td>Low-permeability host rock most important barrier. Importance of EBS increased if there is groundwater flow.</td>
<td>EBS important. Cementitious materials limit groundwater flow and provide long-lasting alkaline conditions.</td>
</tr>
<tr>
<td><strong>Secondary barriers</strong></td>
<td>Alkaline and reducing environment due to cementitious materials will limit radionuclide solubility and increase sorption.</td>
<td>Alkaline and reducing environment due to cementitious materials will limit radionuclide solubility and increase sorption.</td>
<td>Host rock with low hydraulic conductivity.</td>
</tr>
<tr>
<td><strong>Waste packages</strong></td>
<td>Concrete (or bitumen) used as immobilisation matrix. Emplacement packages often proposed.</td>
<td>Several immobilisation matrices proposed. Cement often used to provide alkaline conditions.</td>
<td>Cement conditioned wastes placed in metal containers or concrete packages.</td>
</tr>
<tr>
<td><strong>Backfill</strong></td>
<td>Grout backfill sometimes used. Seals prevent parts of repository from forming gas pathways.</td>
<td>Rock bolts and grout (sometimes bentonite) backfill often used for mechanical stability.</td>
<td>Crushed rock used to divert flow away from waste packages.</td>
</tr>
</tbody>
</table>

Table 2.2: Common features of ILW repositories in different geological settings (based on Hicks et al., 2008).
of C-14 from the repository by filling the crown space with a suitable material such as anthracite slurry. However, sorption depends on the partial pressure of methane and CO\textsubscript{2} rather than the total pressure and, as the bulk of the gas is expected to be hydrogen, the partial pressures of CH\textsubscript{4} and CO\textsubscript{2} may be too small.

In the Belgian ILW repository concept, the wastes are conditioned in cement or bitumen in 200 or 400-litre steel drums. The waste packages are then placed in pre-fabricated concrete monoliths, which will keep the dose rate outside the monoliths below a predetermined rate and provide a hydrological and chemical barrier. The monolith is expected to provide a barrier to groundwater movement and additionally concrete will provide a high pH environment in which the corrosion of steels is low. The use of monoliths could be applied to the UK concept, but the increased volumetric requirements may prove to be problematic (Hicks et al., 2008).

2.5 Discussion

This chapter introduced the UK disposal concept and how it is designed to contain radionuclides. The processes that generate gas within the facility after its closure were also described. The radioactive waste inventory contains materials with the capability to produce large quantities of gas. The majority of the gases produced after the repository has been closed will be generated as a result of corrosion. Some radioactive gas may, however, also be formed, which is why gas migration from the repository needs to be considered in safety assessments.

The migration of gases depends on the properties of the host rock, the repository design and the materials used within the repository. As the different potential host rocks are known, and initial repository designs for them have been prepared, scoping calculations can be performed to determine the possible effects of gas generation and migration. The following chapters explain how numerical modelling can be used to estimate whether gases escape from the repository and their behaviour as they move through the host rock. Chapter 3 introduces the laws governing fluid transport in porous media, and Chapter 4 explains what has already been done to investigate the problem. The remaining chapters then use numerical modelling as a tool to demonstrate what happens to the repository gases, and to investigate whether it is possible to manage these processes through the design of the disposal facility.
Chapter 3

Gas Migration Theory

This chapter considers the mathematical representation of fluid flow in porous media. The chapter starts by explaining how gases are expected to behave in the pressurised two-phase environment. Laws governing compression and dissolution are given, and concepts important to two-phase flow, such as wettability and capillary pressure, are introduced.

The mathematical expressions for fluid transport are then discussed. Advective flow is expected to be the main transport mechanism for gases in many host rocks. Advection refers to the fluid’s bulk motion in a particular direction, and can be described using Darcy’s Law. Section 3.2 discusses the application of Darcy’s Law to two-phase flow problems, and the limitations of the theory. The concept of relative permeability is considered in depth, as it can have a large impact on the accuracy of multiphase flow studies.

Diffusion describes the spontaneous transport of particles from regions of higher concentration to regions of lower concentration. Diffusive flow may become the dominant transport process in very low permeability rocks. The mathematics of hydrodynamic dispersion, which includes diffusion, are considered in Section 3.3.

The chapter ends by explaining some of the concepts used in numerical modelling of multiphase flow. First, the mass balance equation for a multiphase system is discussed. Mass balance equations are used to predict mass flows within a system. The concluding section discusses some of the factors which introduce uncertainties in gas migration modelling, including for example chemical and physical processes affecting groundwater flow, fracturing of the host rock and coupled phenomena. A brief discussion on upscaling techniques is also provided.
3.1 Behaviour of gases in pressurised environments

The repository will be ventilated during its operational phase, and any gases generated by the wastes will be removed. Inflowing groundwater will also be removed by pumping. After closure, groundwater will start to flow into the repository from all directions and fill empty pore space within its structures. This flow is driven by the pressure gradient caused by the difference between the atmospheric pressure in the repository and the hydrostatic pressure around it. The pressure gradient is initially large, but it reduces as more and more water enters the repository and the repository pressure increases. The groundwater inflow rate will therefore reduce over time.

A pressure drawdown area is likely to form around the repository during its operational phase. The extent of the drawdown area will depend on the repository depth and materials, and the properties of the host rock. As well as flow into the repository, local flow inside the repository will occur due to the height differences within the repository structures.

Air retained in the repository from the operational phase will compress as the repository pressure increases. Inflowing groundwater starts gas generation processes within the disposal vaults, thus increasing the total amount of gas in the repository. Some of the gas will dissolve in the groundwater, but a free gas phase is also likely to form. This will further increase the pressure in the repository. This section explains the expected behaviour of gases in the repository setting and introduces some concepts important to gas migration. These are, for example, capillary pressure and soil water characteristic curves.

3.1.1 Volume of gases

The volume of gases in pressurised environments changes according to Boyle’s Law. Boyle’s Law states that the volume of an ideal gas is inversely proportional to the gas pressure at a constant temperature. The maximum volume of gases in repository conditions \( V_g \) can therefore be estimated from

\[
V_g = \frac{1 \cdot 10^5 \text{Pa}}{P_g} V_{STP}
\]

if the pressure at the repository depth, \( P_g \) (in Pa), and the volume of gases in STP conditions, \( V_{STP} \) (in m\(^3\)), are known. Boyle’s Law is expected to hold fairly well for
repository gases, as temperatures and pressures encountered are moderate (see for example Nirex, 2003b).

Using Boyle’s Law, the maximum pressure in the repository at early times, when gases are not yet able to flow out, can be calculated. The pressure should be kept sufficiently low to prevent fracturing of the host rock.

### 3.1.2 Solubility of gases

As the pressure in the repository increases, more and more gas will dissolve. The solubility of repository gases in groundwater is governed by Henry’s Law. Henry’s Law states that, at a constant temperature, the amount of a gas dissolved in a given type and volume of liquid is directly proportional to the partial pressure of the gas in equilibrium with the liquid.

\[ H_L = \frac{C_x}{P_x} \]  

(3.2)

where

- \( H_L \): Henry’s law constant \( (\text{kg} / (\text{m}^3 \cdot \text{atm})) \)
- \( C_x \): equilibrium concentration of the gas in solution \( (\text{kg}/\text{m}^3) \)
- \( P_x \): partial pressure of gas \( (\text{atm}) \)

Henry’s constants for some of the gases commonly encountered in repository conditions are presented in Table 3.1.

<table>
<thead>
<tr>
<th>Gas</th>
<th>Solubility at 25°C, 1 atm partial pressure (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_2 )</td>
<td>( 1.5 \times 10^{-3} )</td>
</tr>
<tr>
<td>( CO_2 )</td>
<td>( 1.4 )</td>
</tr>
<tr>
<td>( CH_4 )</td>
<td>( 2.1 \times 10^{-2} )</td>
</tr>
</tbody>
</table>

Table 3.1: Henry’s constants for common repository gases (from Dean, 1999).

Fetter (1999) states that Henry’s Law is valid if the gas phase is sparingly soluble, reasonably ideal and will not react with the solute. Solubility is also affected by salinity and temperature. At higher temperatures, or in areas of higher salinity, less gas will dissolve. As groundwater flows through the host rock, the pressure, temperature and
salinity conditions it experiences vary. Some of the gas may come out of solution, or more gas may be able to dissolve.

### 3.1.3 Gas transport

Gases may migrate out of the repository in both liquid and gaseous phases. During the resaturation phase, gases in the repository will initially be prevented from entering the surrounding host rock due to the large pressure gradient directed towards the repository. As the pressure gradient decreases, the gases will at some point become able to migrate out. As they leave the repository, the repository pressure may fall sufficiently for the gas pathway to close until further gas generation results in the gas entry pressure being exceeded again. The rate of gas outflow may therefore fluctuate.

![Figure 3.1: Gas may migrate out of the repository in both liquid and gaseous phases.](image)

Advective and diffusive flows transport gases through the host rock. The rate at which gases are transported depends on the properties of the rock and the pressure and concentration gradients, as will be discussed in Sections 3.2 and 3.3. Before moving on to these topics, however, the following sections explain some of the key concepts required for understanding multiphase fluid flow.
3.1.3.1 Wettability

Wettability is the preference of a solid to contact one liquid or gas, known as the wetting phase, over another. A water-wet rock would have much more affinity for water than gas, and a large part of the rock surface would be covered with a thin water layer. The wetting phase, here water, tends to moisten as much grain surface as possible due to its surface tension. The other fluid, here gas, is the non-wetting phase which flows preferably in the middle of the pore spaces and forms bubbles or a continuous phase. This is demonstrated in Figure 3.2. Wettability affects relative permeability and capillary pressure.

![Figure 3.2: An illustration of gas and water phases between soil particles.](image)

3.1.3.2 Capillary pressure

In a gas-water system, there is a discontinuity in fluid pressures across the interface between the two fluids. This is called the capillary pressure, and it results from the interfacial tension, the wetting characteristics of the rock and the curvature of the interface. Capillary pressure, $p_c$, represents the difference between gas and water pressures, and can be expressed as:

$$p_c = P_g - P_w$$  \hspace{1cm} (3.3)
where $P_g$ is the gas phase pressure and $P_w$ is the water phase pressure. Capillary pressure controls two-phase flow as it introduces a gas entry pressure which needs to be overcome before water will be displaced from an initially fully saturated medium. Once the gas entry pressure has been exceeded, gas flow is controlled by the permeability of the rock, the relative permeability and the saturation-capillary pressure relationship as discussed below.

Capillary pressure depends on the saturation and the saturation history of the system. Capillary pressure curves describe the capillary pressure required to obtain a given saturation for the non-wetting phase. Figure 3.3 shows a typical capillary pressure curve for a water-gas system in a porous rock. The curve consists of three parts: first drainage, first imbibition and second drainage. During the drainage phase, water is displaced from a mainly water-filled medium by gas. Imbibition refers to the phase during which water returns to the system and displaces gas from the now water and gas containing system. These processes are explained below.

![Capillary Pressure Curve](image.png)

Figure 3.3: A typical capillary pressure curve, shown as a function of water saturation, $S_w$. 

1. First drainage
2. First imbibition
3. Second drainage
3.1. BEHAVIOUR OF GASES IN PRESSURISED ENVIRONMENTS

First drainage

At water saturation $S_w = 1$ (i.e. when all the pores only contain water), an entrance pressure, $P_0$, called the ‘threshold pressure’ or ‘gas entry pressure’ needs to be exceeded before gas can enter the system. A plateau is then reached. At decreasing water saturations, increasing amounts of pressure are needed to force water out from the smaller and smaller pores. The capillary pressure rises to infinity at the connate water saturation $S_{cw}$, i.e. the lowest water saturation found in situ. The remaining water is trapped within the system and cannot be forced out.

First imbibition

When the gas pressure is decreased, water will spontaneously imbibe and the saturation increases. The capillary pressure decreases and remains smaller than the drainage capillary pressure. This is because the surface tension of water is now dominated by the large pores, while during drainage the surface tension of water in the small pores is the dominating factor. When the gas pressure is equal to the water pressure, the saturation reaches the spontaneous water imbibition saturation $S_{spw}$. Water can now be added by increasing the water pressure above that of the gas. By definition, the capillary pressure becomes negative. Increasingly high water pressures are required to force the remaining gas out until the residual gas saturation $S_{gr}$ is reached, at which point the capillary pressure goes to minus infinity. At the residual gas saturation, gas no longer forms a connected phase and becomes immobile within the system.

Second drainage

When the water pressure is slowly decreased again, gas will spontaneously imbibe and the saturation decreases. The capillary pressure increases and, due to hysteresis, is generally higher than the imbibition capillary pressure for the same saturation. At $S_{spg}$ the spontaneous gas imbibition stops. A further increase in the gas pressure leads to a decrease in the water saturation, until at $S_{cw}$ the capillary pressure again becomes infinitely large.

The time at which gases start to flow out of the repository depends on the capillary entry pressure of the host rock. This barrier pressure may be very large for a host rock with small pores, such as clay or mudstone. Once the capillary entry pressure has been overcome, and a gas pathway becomes established, the capillary barrier no longer needs to be overcome in order for gases to flow out.

A soil water characteristic curve (SWCC) is a curve based on experimental data or
statistical prediction which describes the relationship between the suction for the soil (i.e. capillary pressure), and the soil water content (i.e. saturation). These curves are needed in numerical assessments of two-phase flow. The most used curve is the drying curve, which depicts the changes in suction when saturation is reduced from 1 to the value for residual saturation.

Figure 3.4 shows a typical SWCC. These graphs are normally drawn with saturation on the vertical axis and soil suction on the horizontal axis, while the convention for capillary pressure curves (see Figure 3.3) is to show pressure on the vertical axis and saturation on the horizontal axis. Figure 3.4 shows how, at first, nearly all pores are filled with water. At the gas-entry value, gas starts to enter the largest pores in the system. Increasing the matric suction results in more water draining out until the residual air content is reached. Thereafter high changes in suction are required in order to remove more water. The shape of the curve is affected by the type of soil: the smaller the grain size, the larger the required suction pressure.

![Figure 3.4: A typical SWCC curve (image taken from Fredlund and Xing, 1994, p. 522).](image)

Several researchers have proposed models to predict the relationship between suction and saturation using general fitting parameters. The three fitting parameters commonly used to describe a SWCC are $\alpha$, $n$ and $m$. Parameter $\alpha$ is a fitting parameter representing the air entry pressure (with units of Pa$^{-1}$), and it is related to the size of the larger pores. Unitless fitting parameters $n$ and $m$ describe the slope of the SWCC and the symmetry of the curve respectively. Both $n$ and $m$ are related to the pore-size distribution of the soil. Some of the most notable models were proposed by Gardner (1958), Brooks and Corey (1964) and Fredlund and Xing (1994). However, perhaps the
most common model using all three fitting parameters was proposed by van Genuchten (1980). He noticed that, in order to avoid complicated mathematical expressions, parameters \( n \) and \( m \) could be related. Therefore, the final equation proposed by van Genuchten (1980) only uses two fitting parameters and is:

\[
S = \left[ \frac{1}{1 + |\alpha \cdot \psi|^n} \right]^{1 - \frac{1}{n}}
\]  

(3.4)

where \( \psi \) is the matric suction head.

### 3.2 Advective flow

It is difficult to predict the behaviour of fluids at large scale. At the pore level, the capillary forces between the fluids and the rock, as well as the wetting characteristics of the rock, can be described. Problems arise when attempts are made to describe multiphase flow at the macro-scale, as the non-uniform pore structure needs to be taken into account. A large number of equations would therefore be required for an accurate representation. Simple expressions describing the fluid behaviour at the larger scale are, however, needed in numerical assessments of fluid flows. This section discusses a mathematical expression often used to estimate advective flow in a porous medium, Darcy’s Law, and its limitations, paying particular attention to the concept of relative permeability.

#### 3.2.1 Darcy’s Law

Darcy’s Law (Darcy, 1856) is often used to estimate fluid flow through a porous medium. It assumes a linear relationship between the fluid velocity and the friction forces experienced by the fluid.

In the 19th century, Henry Darcy formulated an expression for advective flow through a saturated porous medium using the experimental set up shown in Figure 3.5. Here, a cylinder with a cross-sectional area \( A \) (in m\(^2\)) is filled with sand and held between two gauze screens. Water flows through the cylinder at a steady rate \( Q_w \) (in m\(^3\)/s). The head loss over a distance \( l \) (in m) is measured. Henry Darcy found that the flow rate is directly proportional to the hydraulic gradient \( dh/dl \) and the cross-sectional area of the cylinder, i.e.
CHAPTER 3. GAS MIGRATION THEORY

Figure 3.5: The experimental set up used to formulate Darcy’s Law.

\[ Q_w = -KA \frac{dh}{dl} \]  

(3.5)

where \( K \) is a constant of proportionality called the hydraulic conductivity with units of m/s. The negative sign indicates that the flow is in the direction of decreasing hydraulic head. This equation can also be written as

\[ q = -K \frac{dh}{dl} \]  

(3.6)

where \( q \) is the specific discharge with units of m/s. \( K \) can then be calculated using the experimental values for \( q \) and \( dh/dl \). The hydraulic conductivity takes into account both the properties of the porous medium and those of the fluid(s) filling it. The properties of the fluid and rock can be separated by using the concept of intrinsic permeability, \( k \) with units of m\(^2\), instead of the hydraulic conductivity.

\[ k = K \frac{\mu}{\rho g} \]  

(3.7)

where \( \mu \) is the dynamic viscosity of the fluid (in Pa \( \cdot \) s) and \( \rho \) is its density. Both \( K \) and \( k \) are functions of temperature. (Note - this thesis deals primarily with multi-phase fluid flows and the use of fluid-dependent hydraulic conductivity is therefore avoided. For the benefit of those readers with an engineering background, the intrinsic permeability of 1 m\(^2\) is approximately the same as the hydraulic conductivity of \( 1 \times 10^7 \) m/s for water.)
3.2. **ADVECTIVE FLOW**

Intrinsic permeability represents the properties of the porous medium that allow fluids to flow through it. These are, for example, porosity and the size distribution and interconnectedness of the pores.

Intrinsic permeability has units of m$^2$ or darcy. Darcy is defined as the permeability that permits 1 ml of fluid of 1 centipoise viscosity, completely filling the pores of the medium, to flow in 1 s through a cross-sectional area of 1 cm$^2$ under a gradient of 1 atm/cm along the flow path. 1 darcy = 1 × 10$^{-8}$ cm$^2$.

The complete expression for single phase flow is now:

$$Q_w = -k\frac{\rho g}{\mu} A \frac{dh}{dl}$$  \hspace{1cm} (3.8)

where

- $Q_w$: discharge (m$^3$/s)
- $k$: permeability (m$^2$)
- $\rho$: density of fluid (kg/m$^3$)
- $g$: gravitational acceleration (m/s$^2$)
- $\mu$: viscosity of fluid (Pa·s)
- $A$: cross-sectional area (m$^2$)
- $dh/dl$: hydraulic gradient (m/m)

### 3.2.2 Two-phase advective flow

The validity of Darcy’s Law has been tested in laboratory experiments, and later experiments have confirmed that Darcy’s Law with minor modifications can also be used to describe the flow of fluids other than water. In systems which contain several types of fluids, the flow of one fluid is affected by the presence of the other fluids (see Sections 3.1.3.1 and 3.1.3.2). The multiphase version of Darcy’s Law can be used to evaluate the transport of water and gas out of the repository and in the host rock:

$$F_\beta = -k_{r_\beta}\frac{\rho_\beta}{\mu_\beta} \left( \nabla P_\beta - \rho_\beta g \right)$$  \hspace{1cm} (3.9)

where

- $F_\beta$: mass or heat flux (kg/(m$^2$·s))
- $k_{r_\beta}$: relative permeability to phase $\beta$
- $\rho_\beta$: density of phase $\beta$ (kg/m$^3$)
\[ \mu_\beta \text{ viscosity of phase } \beta \text{ (Pa \cdot s)} \]

\[ P_\beta \text{ fluid pressure in phase } \beta \text{ (Pa)} \]

This expression includes a term for relative permeability, \( k_{r,\beta} \), which expresses the permeability of the media to a certain type of fluid in the presence of other fluids, in order to account for their simultaneous flow. The difference between permeability and relative permeability is explained below.

**Permeability**

Permeability is a rock property which expresses the ease with which any fluid may penetrate the rock matrix. The intrinsic permeability of rocks is caused by the primary openings formed within the rock and secondary openings created after the rock was formed. The percentage of void space within rock is called porosity. The porosity, size of the pores and the degree to which they are connected all affect permeability. Most rocks are heterogeneous, and their permeability is also often dependent on the direction; this is called anisotropy. Anisotropy arises from the fact that most rock grains are not spherical, and they tend to settle so that shorter axes point in the vertical direction during deposition.

**Relative permeability**

Relative permeability is a fluid property which expresses the permeability as the fluid would see it in the presence of other fluids. The presence of other fluids makes movement more difficult, and the effective permeability for the fluid is therefore smaller than the permeability of the rock. Permeability has units of length squared, while relative permeability is expressed as a fraction.

Relative permeability has been a subject of scientific research since the start of the 20th century. However, there are still areas of uncertainty. The representation of relative permeability in numerical assessments is currently one of the factors with a significant impact on the accuracy of results.

### 3.2.2.1 Relative permeability

Figure 3.6 shows a simple, but unrealistic, way of approximating relative permeability for a system with two fluids. Here, relative permeability is expressed as a function of the saturation of the wetting phase. Linear relative permeability curves assume that the mobility of each phase is a linear function of the saturation, and no cut-off
3.2. **ADVECTIVE FLOW**

points where one of the fluids becomes fully mobile or immobile are present. They also consider both phases to be independent of each other. The solid line represents the relative permeability of the wetting phase, e.g. water, and the dashed line the relative permeability of the non-wetting phase, e.g. gas. When only water is present, i.e. saturation equals 1, the relative permeability of water is 1. However, in the presence of gas, the relative permeability reduces linearly, until the only fluid present is gas (saturation = 0), at which point the relative permeability of gas reaches unity.

![Figure 3.6: A possible (but inaccurate) way of approximating relative permeability as a function of the wetting phase saturation. The solid and dashed lines represent the wetting and the non-wetting phases respectively.](image)

In reality, the mobility of each phase is severely retarded by the presence of the other, so that the sum of the relative permeabilities never reaches 1. Relative permeability functions are often quadratic and a much more realistic scenario is presented in Figure 3.7. As the saturation of the wetting phase (solid line) reduces, the fluid is confined to smaller and smaller pores. Flow becomes restricted, due to the reduction in volume through which flow occurs and the increase in capillary pressure (see Section 3.1.3.2). A small change in saturation can therefore have a large effect on relative permeability. It can be noticed that the relative permeability of the wetting phase remains low unless the system is fully saturated. One of the reasons for this is that the wetting phase is in contact with the pore surface and experiences much higher friction forces than the non-wetting phase. Thus, above a certain saturation, the wetting fluid reaches its peak relative permeability. The effective permeability is, however, only a fraction of the
permeability. At very small saturations, the relative permeability of the wetting phase drops to zero. This occurs when the fluid no longer forms a connected (i.e. continuous) phase, but sits at the pore throats and small openings on the surface, or when it is so thinly spread over the rock grains that the friction forces are too large to allow flow.

\[ \text{Figure 3.7: The relationship between relative permeability and saturation in a two-phase system.} \]

The relative permeability of the non-wetting phase reaches values much closer to one at small saturations, i.e. when the fluid forms a continuous phase in the ‘middle’ of the pore space and flows freely. The curve drops to zero when the saturation is so large that only immobile bubbles are left in the pore spaces.

### 3.2.2.2 Relative permeability functions

Several authors have derived relative permeability - saturation functions. The relationship between relative permeability and saturation can be determined using laboratory experiments in which fluids are injected through a small core, or by using field data. Relationships obtained from field data suffer from inaccuracies due to the number of assumptions that need to be made regarding the uniform structure of the medium and its water saturation. Laboratory experiments provide the most reliable results, but carry errors due to boundary effects which cause changes in pressure and saturation on the core edges. Additionally, the fluid behaviour greatly depends on the rock properties. Empirical curves are therefore estimates which are only valid for the particular
A large number of empirical relative permeability - saturation curves are available for different fluids and rock types (see for example Fredlund and Xing, 1994; Leong and Rahardjo, 1997). While the most relevant one should be selected for any numerical study, its validity in different conditions - including but not restricted to temperature, pressure and chemical composition of rocks and fluids - should always be questioned. The three relative permeability functions used in this thesis are presented below in the order of increasing complexity. Other models, such as those proposed by Gardner (1958), Brooks and Corey (1964) and Fredlund and Xing (1994), are available, but have been found to produce less accurate results or require the use of more than two fitting parameters.

**Linear functions**

As discussed above, linear functions assume that the relative permeability of water increases linearly from 0 to 1 as the water saturation of the system increases from the user-defined value for irreducible water saturation, $S_{lr}$, to 1. Similarly, the relative permeability of gas reduces from 1 to 0 as the gas saturation reduces from 1 to the user-defined value for irreducible gas saturation, $S_{gr}$. Figure 3.8 shows an example where the irreducible water and gas saturations are taken to be 0.3 and 0.001 respectively.

![Linear relative permeability curve](image-url)
Corey’s function

Corey’s function (Corey, 1954) also requires the irreducible liquid and gas saturations as input. The function is expressed as:

\[
\begin{align*}
  k_{rl} &= \hat{S}^4 \\
  k_{rg} &= (1 - \hat{S})^2 (1 - \hat{S}^2)
\end{align*}
\]

where

\[
\hat{S} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}
\]

Figure 3.9 shows an example of Corey’s relative permeability curve, where the irreducible water and gas saturations are taken to be 0.3 and 0.001 respectively.

![Corey's relative permeability curve](image)

Figure 3.9: Corey’s relative permeability curve, with user-defined values of $S_{lr} = 0.3$ and $S_{gr} = 0.001$.

Van Genuchten function

As discussed in Section 3.1.3.2, the relationship between saturation and capillary pressure can be described using empirical models. A linkage between relative permeability and capillary pressure therefore also exists. Mualem (1976) and van Genuchten (1980) developed a statistical model based on the idea that both the SWCC and the relative permeability function are related to the pore size distribution, and the same fitting
parameters, $\alpha$ and $n$, can be used for both functions. The van Genuchten-Mualem function takes the following form:

\[
k_{rl} = \begin{cases} 
\sqrt{S^*} \left\{ 1 - \left[ 1 - (S^*)^{1/\lambda} \right]^\lambda \right\}^2 & \text{if } S_l < S_{lr} \\
1 & \text{if } S_l \geq S_{lr}
\end{cases}
\]

\[
k_{rg} = \begin{cases} 
1 - k_{rl} & \text{if } S_{gr} = 0 \\
(1 - \hat{S})^2(1 - \hat{S}^2) & \text{if } S_{gr} > 0
\end{cases}
\]  

(3.11)

where

\[
0 \leq k_{rl}, k_{rg} \leq 1 \\
S^* = \frac{S_l - S_{lr}}{S_{ls} - S_{lr}} \quad \text{and} \quad \hat{S} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}
\]

(3.12)

Liquid and gas saturations are denoted by $S_l$ and $S_g$, and irreducible liquid and gas saturations by $S_{lr}$ and $S_{gr}$ respectively, while $\lambda$ is a shape parameter ($\lambda = 1 - 1/n$). The exact shape of the curves and their cut-off points are defined by the user depending on the type of rock and fluids. Mualem (1976) and van Genuchten (1980) compared their results with observed hydraulic conductivities of different soils and found that the calculated expression followed closely the observed data in four out of five cases. The function proposed by Mualem and van Genuchten is now widely used in numerical modelling due to the simplicity of using the same fitting parameters for both functions, and the fact that only two parameters are required without over-compromising on accuracy. An example van Genuchten relative permeability curve is shown in Figure 3.10 where the following parameters are used: $S_{lr} = 0.3$, $S_{gr} = 0.001$ and $\lambda = 0.5$.

The van Genuchten capillary pressure function is expressed as:

\[
p_c = -P_0(\left[ S^* \right]^{-1/\lambda} - 1)^{1-\lambda}
\]

(3.13)

An example capillary pressure curve is shown in Figure 3.11, with $S_{lr} = 0.3$, $\lambda = 0.5$ and $P_0 = 2 \times 10^6$. 

Understanding that Darcy’s Law is only an approximation of the forces influencing the fluid flow, and that there are many limitations to it, is vital. Some of the uncertainties in numerical modelling employing Darcy’s Law arise from the following:

- Darcy’s Law assumes laminar flow. At higher velocities - e.g. when the pore sizes or flow velocities are large - turbulent flow conditions may prevail and the law is no longer valid.

- For environments with very low permeabilities, advective flow becomes insignificant in comparison with diffusive flow. This is considered further in Section 3.3. For very low permeability environments, Darcy’s Law may also become invalid due to the increased friction forces between the very small pores of the rock and the fluid.

- It is difficult to express a complicated heterogeneous system with only one parameter representing permeability as pore sizes and connectivities are not constant. Permeability can vary by several orders of magnitude within short distances, while areas studied are often much larger.

- Relative permeability curves change with the type of fluids, materials and conditions used in the experiment. While it is important to understand relative permeability curves, and to develop accurate relationships, it is unlikely that perfect information will ever become available. This is because the large scale
fluid flow seen in nature, or in laboratory experiments, does not give information about the micro-scale behaviour that takes place in the rock pores. Describing this behaviour accurately on a large scale would be hugely complicated, due to the varying pore sizes and connectivities, wetting behaviour of the rock, miscibility of the fluids, etc. Instead it needs to be understood that numerical assessments always carry errors, relative permeability being one of them.

- Another complication arises from the miscibility of the fluids: Relative permeability - saturation relationships are commonly used in petroleum engineering, and curves for oil-water and oil-gas systems determined in laboratory experiments are available. It has been determined that for immiscible fluids only one fluid flows through a given pore at a time. The behaviour of miscible fluids is, however, less well understood, as simultaneous flow may occur. The miscibility of different gases therefore needs to be understood before migration studies can be carried out.

### 3.3 Hydrodynamic dispersion

Fluids will not flow from place A to place B by taking the shortest route; dispersion occurs. Figure 3.12 shows the dispersion of a solute slug that is being advected with groundwater. Over time the concentration of the solute reduces as more and more dispersion takes place.

![Figure 3.11: Van Genuchten capillary pressure curve, with $S_{lr} = 0.3$, $\lambda = 0.5$ and $P_0 = 2 \times 10^6$.](image-url)
3.3.1 Diffusion

In very low permeability environments, where groundwater flow is extremely slow, diffusion may be the dominant process by which dissolved gases move through the medium. Diffusion is a process which causes dissolved gases to move from areas of high concentration to areas of lower concentration due to the random thermal motion of molecules and ions. Steady-state diffusion is often described using Fick’s Law:

\[ F = -D \nabla C \]  \hspace{1cm} (3.14)

where

- \( F \) - diffusional flux of solute (mol/(m\(^2\)·s))
- \( D \) - diffusion coefficient (m\(^2\)/s)
- \( C \) - concentration of a species (mol/m\(^3\))

If the concentration of the solute changes with time, Fick’s Second Law may be applied:

\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \]  \hspace{1cm} (3.15)
3.3. HYDRODYNAMIC DISPERSION

The value of the diffusion coefficient, \( D \), depends on the type of species, temperature, pressure and interactions with other species. Typical values for some of the common repository gases are presented in Table 3.2.

<table>
<thead>
<tr>
<th>Gas</th>
<th>Diffusion coefficient ((\times 10^{-9} \text{m}^2/\text{s}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_2)</td>
<td>5.11</td>
</tr>
<tr>
<td>CO(_2)</td>
<td>1.91</td>
</tr>
<tr>
<td>CH(_4)</td>
<td>1.84</td>
</tr>
</tbody>
</table>

Table 3.2: Diffusion coefficients for typical repository gases (from Lide, 2000).

In porous media, diffusion processes transport molecules slower than in water due to the presence of mineral grains. The effective diffusion coefficient, \( D^* \), is therefore used:

\[
D^* = wD
\]  

(3.16)

where \( w \) is an empirical coefficient whose value ranges from 0.01 to 0.5 (Freeze and Cherry, 1979). Porosity and tortuosity are among the factors said to affect the magnitude of \( w \). In a two-phase system, the diffusion coefficient is defined as:

\[
D^*_\kappa = \phi \times \tau_0 \times \tau_\beta \times d^*_\kappa
\]  

(3.17)

where \( \phi \) is porosity, \( \tau_0 \times \tau_\beta \) is tortuosity which is dependent on the properties of the porous medium \( (\tau_0) \) and phase saturation through \( \tau_\beta = \tau_\beta(S_\beta) \), and \( d^*_\kappa \) is the molecular diffusion coefficient for component \( \kappa \) in phase \( \beta \).

3.3.2 Mechanical dispersion

As groundwater containing dissolved gases from the repository flows through a porous medium, it will mix with groundwater in its natural state. This results in the dilution of the dissolved gases, known as mechanical dispersion. Mechanical dispersion occurs due to the heterogeneities of the porous medium. The mixing occurring in direction of the fluid flows is called longitudinal dispersion, while dispersion normal to the fluid flow is called transverse dispersion.

Longitudinal dispersion occurs due to the fact that fluids flow through the large pores faster than through the small pores, and through the middle of the pore spaces faster than along the edges. Transverse dispersion is caused by the branching out of the flow.
path. Longitudinal dispersion is normally much greater than transverse dispersion.

### 3.3.3 Hydrodynamic dispersion

By combining the expressions for diffusion and mechanical dispersion, hydrodynamic dispersion can be expressed as:

\[
D_L = a_L v_x + D^* \tag{3.18}
\]

where

- \(D_L\) longitudinal coefficient of hydrodynamic dispersion
- \(a_L\) dynamic dispersivity
- \(v_x\) average linear groundwater velocity
- \(D^*\) effective molecular diffusion coefficient

The one-dimensional hydrodynamic dispersion equation is given by

\[
D_L \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \tag{3.19}
\]

This equation assumes that the solute is moving at the same advection flow rate as groundwater, but that dispersion causes the solute to spread out ahead and behind the groundwater front, as shown in Figure 3.13.

### 3.4 Mass balance equation

The previous sections introduced expressions for estimating fluid fluxes due to advection and hydrodynamic diffusion. To accurately model the mass flows within a system, a mass balance equation for each component present is needed.

The mass conservation law is used to identify mass flows, by accounting for material entering and leaving. The basic mass balance equation is:

\[
\frac{d}{dt} \int_{V_n} M^s dV_n = \int_{\Gamma_n} \mathbf{F}^s \cdot \mathbf{n} d\Gamma + \int_{V_n} q^s dV_n \tag{3.20}
\]

where

- \(V\) volume in question
3.4. MASS BALANCE EQUATION

Figure 3.13: Breakthrough of a solute. Some of the solute can be detected ahead and behind the groundwater front.

\[\begin{align*}
\Gamma & \quad \text{boundary surface} \\
M & \quad \text{mass or energy per volume} \\
\kappa & \quad 1...\text{MK mass component} \\
\kappa & \quad \text{NK+1 heat component} \\
F & \quad \text{mass or heat flux} \\
n & \quad \text{vector normal to the boundary surface, pointing inwards into the volume in question} \\
q & \quad \text{sink/source}
\end{align*}\]

This indicates that the rate of change of mass within the observed volume, over a given period of time, is the summation of two components: the net mass flux through the boundary surface and the mass generated within the volume. The mass accumulation term can be calculated from:

\[M^\kappa = \phi \sum_\beta S_\beta \rho_\beta X_\beta^\kappa\] (3.21)

where

\[\begin{align*}
\phi & \quad \text{porosity} \\
S_\beta & \quad \text{saturation of phase } \beta \\
\rho_\beta & \quad \text{density of phase } \beta
\end{align*}\]
$X_\beta^\kappa$ mass fraction of component $\kappa$ present in phase $\beta$

The total mass of component $\kappa$ is obtained by summing over all the fluid phases (e.g. liquid, gas).

It is assumed that all phases are in thermodynamic equilibrium. The number of thermodynamic degrees of freedom can be obtained from Gibb’s phase rule:

$$f = NK + 2 - NPH$$

(3.22)

where $NPH$ is the number of phases and $NK$ is the number of components. Additionally there are saturation degrees of freedom, the number of which is equal to $(NPH - 1)$. The total number of degrees of freedom in the system is therefore:

$$NK1 = f + NPH - 1 = NK + 1$$

(3.23)

This implies that, in numerical modelling, $NK$ mass balance equations and one energy balance equation per grid block are needed to solve the state of the system at any time.

### 3.5 Discussion

This chapter discussed numerical techniques for modelling multiphase fluid flow through porous media. The expressions introduced in the chapter will later be used to model the behaviour of repository gases.

The previous sections showed that gas transport is controlled by the microscopic properties of the porous medium. Numerical gas migration studies, however, require simplified expressions for fluid flow. For example, homogeneous material properties are assumed, even though properties such as permeability may have large variability. This results in large uncertainties. It was also indicated that the choice of capillary pressure and relative permeability functions is vital for numerical assessments. The flow of gases out of the repository is, however, not only dependent on the porous medium and fluid properties in question. It is also strongly affected by other phenomena, such as possible fracturing of the host rock, and chemical and physical reactions taking place between the fluid and solid phases. The next sections briefly explain some of the further issues affecting fluid flow and its mathematical representation. These may cause
3.5. DISCUSSION

further uncertainty in the results of gas migration modelling.

3.5.1 Examples of phenomena affecting fluid flow

Some chemical and physical processes can cause retardation of the solute movement. Chemical reactions, such as carbonation of the cementitious materials in the repository, may lead to the reduction of porosity and permeability, and thus a reduced fluid flow rate. Another example of a chemical process affecting fluid flow is adsorption. This occurs when surfaces of solids, particularly clays, have an electric charge which attracts a charged ion in the fluid.

Fracturing of the host rock is a physical process affecting fluid flow. If the repository gases are unable to enter the host rock, the pressure in the repository increases. If the gas pressure then exceeds the strength of the host rock, both microscopic and macroscopic fracturing may occur. Pathway dilation is an important aspect of gas flow in weak low permeability environments such as clay (see for example Horseman, 1996). Clay-rich rocks cannot withstand long-term gas pressures greater than the minimum principal stress acting on the rock mass. If pressure is increased above this level, microfracturing of the rock may occur, leading to an increase in the porosity and permeability of the rock. While new gas pathways are formed, existing fractures may re-seal as the pressure in them drops. Rock properties are therefore no longer constant. Large-scale fracturing may also occur if the gas pressure increases rapidly. The permeability of the newly formed fracture may be several orders of magnitude higher than that of the host rock. Such a situation is, however, unlikely to occur in a repository environment as gas generation processes are gradual.

Gas migration studies are further complicated by the coupling of some of the above mentioned processes. For example, chemical reactions may change the permeability and porosity of the host rock and repository materials. This in turn may lead to increased gas pressures and therefore cause fracturing of the host rock.

3.5.2 Note on upscaling

Gas transport is affected by the microscopic properties of the porous medium. However, properties such as permeability can vary by several orders of magnitude over short distances. Consider the presence of a fault, of width much less than the size of the grid block, in an otherwise low permeability host rock. The permeability of the fault can be
several orders of magnitude higher than that of the rest of the rock. Gas flow is likely to occur primarily through the fault. However, if the material properties of each grid block are taken to be the average of the material properties within the block, gas flow through the fault may not be detected in the model. Flow through the fault would then be replaced by a much slower flow rate through the entire rock matrix, distorting the results considerably.

Upscaling strategies deal with the problem of representing the small-scale material properties that have a large impact on the macroscale behaviour of fluids. Some of the techniques currently in use include the following:

**Statistical approaches**

Material properties are generated using a statistical method and allocated to grid blocks randomly (see for example Phoon, 2008). This is close to the traditional averaging method and grid size has got a large effect on the outcome. Additionally, a large number of runs may be required to test the sensitivity of the model.

**Grid alignment and discretisation**

This is particularly important when the primary direction of flow is not horizontal or vertical. Grid blocks can be aligned with the main direction of fluid flow instead of using blocks in straight vertical and horizontal lines. Smaller elements for areas of importance can also be used. These methods may, however, be time-consuming.

**Local upscaling**

A small-scale ‘experiment’ is carried out to determine the permeability of an interface of high importance to the flow. The permeability can then be used in the large-scale model to determine the general direction of flow. This process can then be repeated iteratively to solve the permeability of the small region taking into account the updated flow direction, and so on. The results using this method look promising (Gerritsen and Lambers, 2008), but extensive pre-processing is required. Local upscaling is used in Chapter 6 to calculate the effective permeability of the repository.
Chapter 4

Gas Migration Modelling

Having introduced the repository concept in Chapter 2 and discussed the mathematical expressions required for representing multiphase fluid flows in Chapter 3, this chapter explains further what this EngD project involves. The chapter starts by discussing the project scope. As gas migration was identified as an area for further research in 2005 (Nirex, 2005), several studies have already been performed to investigate the problem. These studies are briefly summarised in order to provide evidence of gaps in the current state of knowledge.

The chapter also considers the selection of a suitable computer program for modelling gas migration from radioactive waste repositories. A list of potential simulators is provided, and the reasons underlying the selection of a specific program are explained. Some of the capabilities of the selected program are then introduced at the end of the chapter.

4.1 Scope of modelling studies

This EngD project aims to model the migration of groundwater and gases in the repository and the surrounding host rock. The resaturation phase of the repository is modelled in order to find out when the gas generation processes start. The gas production rates are not modelled, but are obtained from previous studies. The groundwater inflow rate affects the gas generation rates, which in turn affect the gas outflow rate. This coupled behaviour is not, however, taken into account in this study. Instead, the emphasis is placed on investigating the effect of different repository designs on the gas migration. Factors such as the permeability of the backfill and liner materials, the thickness of the liner material, the fill material of the crown space and the layout of the repository and waste packages within it are investigated. Fluid transport is also
affected by the mechanical behaviour of the rocks, such as fracturing, and chemical reactions between the fluids and the host rock. These phenomena are not considered in this project.

The repository is assumed to be located in a homogeneous rock mass. The properties of the host rock affect the time it takes for the gases to migrate to the ground surface, the strength of the gas fluxes at the surface, and the area over which gases in both dissolved and gaseous forms can be found after a certain time. The effect of caprocks and faults is investigated in order to improve the understanding of their effect on the above factors. The project does not aim to model the migration of gases in a known geology with detailed features, and thus only generic features are used.

Most of the modelling is performed using 3D models of the repository and the surrounding host rock. Ultimately the results will indicate how the different repository design features affect gas migration, and what impact uncertainty and variability in the properties of those features have on the behaviour of gases. It is hoped that the results can be applied to improve the design of the facility with regards to gas management. The project does not aim to calculate the gas outflow rates and fluxes from a certain type of repository. Nor will it provide accurate predictions of the repository footprint area and the gas breakthrough time on the surface. Instead, the results are used to compare the impact of different repository features.

The location of the repository is still unknown. This results in uncertainty regarding the type of host rock that the repository will be excavated in; possible environments include fractured rock, clay and evaporite (salt) rock, each with different groundwater and gas flow properties. While gas transport may be diffusion dominated in very low permeability rocks such as clay, advection will be the main transport process in fractured rock. Fluid flow in evaporite rock is very different due to the rock being dry and impermeable; fluid flow would therefore only occur due to mechanical deformation of the rock. As programs developed for fluid flow problems rarely cover mechanical changes of the rock, this type of host rock is not covered in this project. Only fractured and clay host rocks are, therefore, considered.

4.2 Previous studies

Most of the work related to numerical assessments of gas migration from nuclear waste repositories has been carried out in the UK and Switzerland. The UK repository was
initially planned to be located in a fractured rock environment through which gases migrate easily. Therefore, gas migration studies performed in the UK aimed to show that radiological exposures and flammability hazards on the ground surface would not occur. In Switzerland, the work has concentrated on proving that the pressure in the repository will not exceed the lithostatic pressure of the host rock. High pressures may result in fracturing of the host rock and the creation of a preferential pathway to the ground surface. The aims of the work carried out in the two countries are therefore fundamentally different. More recently, gas migration has also been studied in many other countries proposing geological disposal.

This section provides brief summaries of the main studies and their conclusions. The results are used to look for gaps in the current state of knowledge and, therefore, to justify further research.

4.2.1 UK

Gas generation is a particularly important issue in the UK due to the large waste inventory and, therefore, the large quantities of gas that can be produced. For this reason, gas generation and migration have been studied intensively in the past couple of years. The NDA have contracted out gas migration assessments to selected contractors, such as Serco. The following paragraphs summarise these studies.

Bate et al. (2008) present the results of gas migration studies of an underground waste repository located in the fractured rock environment at Sellafield. A large 2D area from below the repository to the ground surface was modelled using the TOUGH2 program (see Section 4.3). The aim of the study was to improve understanding of gas migration in the geosphere. The formation of a pressure drawdown area around the repository was modelled, along with the pressure increase in the repository. The gas generation and groundwater flow rates were not fully coupled. The pressure increase in the repository was found to be small enough not to induce fracturing of the host rock. It was also found that, once the pressure in the repository has risen sufficiently, a free gas phase will be able to migrate out of the repository. The migration through the geosphere is then controlled by the hydrogeological properties of the rocks, such as their permeabilities and gas entry pressures. The study showed that many factors controlling gas migration are site-specific, but that repository design also plays an important role.
CHAPTER 4. GAS MIGRATION MODELLING

The most important factors controlling gas migration were found by Bate et al. (2008) to be: the hydrogeological properties of rocks; localisation of gas due to rock properties and features, and thus the amount of groundwater the gas comes into contact with; repository design, which affects the groundwater inflow rate and the amount of gas that can escape with the first pulse; the groundwater flow rate and the quantity of dissolved gas already contained within the groundwater. In most cases studied, free gas did not break through at the surface, but all gas dissolved and moved with the groundwater. The study raises a question of whether break through time is an appropriate measure of gas transport, as it is highly dependent on the rock properties chosen. Measures such as the strength of gas fluxes in and around the repository could be considered instead.

Another, unpublished, report by Bate et al. (2007) presents the results of a study investigating gas migration in the vicinity of a vault situated in a fractured rock environment. Detailed 3D models of vaults and their surroundings, including seals, the Excavation Damaged Zone (EDZ - see discussion in Chapter 6.2.3) and the surrounding host rock, were used. The effects of the crown space, EDZ, grouting and in-situ gas sorption were examined. The gas generation rate and the groundwater inflow rate were again not fully coupled, but different gas generation rates were used for different resaturation times.

The vault modelled by Bate et al. (2007) was 300 m long and had a cross section of 16 m × 16 m. The crown space was assumed to be approximately 6 m high and in some calculations the vault was assumed to have an internal concrete lining of approximately 0.2 m thick. The vaults were assumed to have concrete floors and each end of the vault was assumed to be connected to an access tunnel aligned with the vault. Tunnels were assumed to be 30 m long and have a square cross section with side of 5 m. All vaults and tunnels were assumed to be backfilled. The EDZ was assumed to be 1 m thick and have a permeability enhanced by a factor of 50 in the direction parallel to the axis of the vault or tunnel and in the circumferential direction, but the same permeability as the host rock in the radial direction.

Results by Bate et al. (2007) indicated that the EDZ has little effect on gas migration and that, in the absence of an open crown space, gas migrates out sooner. The presence of a low-permeability liner around the vault was found to reduce the extent of a pressure drawdown area and the groundwater inflow rate, thus affecting the gas generation rate. The effect of a transmissive feature intersecting the vault was also investigated, and it was found that gas migrates out some distance away from the feature while
4.2. PREVIOUS STUDIES

groundwater flows in through the feature.

After the two studies summarised above, it was recognised that carbon-14 is a key issue for repository performance assessments and an update of C-14 migration in gas phase was needed. The report by Hoch et al. (2008) presents the results of gas generation calculations, including the release rates of active gases $^3$HH, $^{14}$CO$_2$ and $^{14}$CH$_4$. Additionally, gas migration calculations were carried out using TOUGH2 and flammability and radiological consequences due to gas release at the ground surface were assessed.

Hoch et al. (2008) concluded that the peak generation rate is approximately $10^6$ m$^3$ per year at STP and that the long term gas generation rate is likely to be $10^2$ - $10^3$ m$^3$/yr. The peak generation rates of $^3$HH and $^{14}$CH$_4$ are approximately 10 TBq per year. $^{14}$CO$_2$ is expected to react with cementitious materials in the repository near field and not migrate to the ground surface.

Hoch et al. (2008) then used three different models: a 1D fractured crystalline host rock model, a 1D clay host rock model and a 2D model based on Sellafield geology. Over-pressurisation was found to be considerable in the clay environment, whereas the pressure increase in the fractured crystalline rock was insignificant. However, the applicability of porous-medium models for gas migration in clay was questioned, as phenomena such as micro-fissuring and fracturing of the rock cannot be taken into account in these models. A large amount of gas was found to dissolve in the groundwater, and therefore certain assumptions, such as the amount of groundwater free gas comes in contact with, were found to affect gas pathway significantly.

All the reports discussed so far considered gas migration through the detailed Sellafield geology. The applicability of the results in other environments could therefore be questioned. Hoch and Swift (2010) identified six generic environments as possible geologies for the UK radioactive waste repository. These were: 1) basement rock to surface; 2) basement rock under sedimentary cover, with permeable sedimentary rocks; 3) basement rock under sedimentary cover, with low-permeability sedimentary rocks; 4) evaporite host rock; 5) mudrock hosted environment; 6) strong sedimentary host rock. Hoch and Swift (2010) assessed the consequences of gas generation for environments 4, 5 and 6. The different vault shapes in different host rocks were taken into account. First, gas generation rates in different host rocks were calculated. It was recognised that the choice of host rock impacts on gas generation rates due to different water inflow rates, backfilling strategies and materials used. The coupling of gas generation to groundwater flow was attempted but simplifications were used. This resulted in
inaccuracies in the estimated gas generation rates.

TOUGH2 was then used by Hoch and Swift (2010) to study gas migration out of the repository. Half of a vault was modelled in each case, and the drawdown area, pressure increase in the repository, flow of gas out of the vault and gas saturation along with the mass fraction of dissolved gas around the repository were calculated at different times. The study found that, in a salt environment, gas does not move a significant distance away from the repository, but instead the pressure in the repository rises. This could cause contaminated water to be driven out of the repository. It was, however, noted that the pressure is unlikely to rise above the strength of the rock. It was also stated that the coupling of gas generation and multiphase flow is difficult and that gas generation may also have an effect on the amount of ‘creep’. In a clay environment and a fractured crystalline host rock, it was found that gas is not retained in the repository near field but migrates through the host rock. This was considered surprising, given the low permeability of the clay host rock.

4.2.2 Switzerland

Nagra, the organisation responsible for radioactive waste disposal in Switzerland, have carried out studies into gas migration from a repository located in a clay environment. Only one report (Nagra, 2008) of the most current work has, however, been translated into English. This report investigates the effects of post-disposal gas generation in a repository for low and intermediate-level waste. Nagra (2008) summarised the state of understanding of gas transport processes in the underground structures of the repository and in the surrounding host rock, and assessed the impact of gas generation on the isolation capacity of the repository.

The use of specially designed backfill and sealing materials is proposed in Switzerland in order to keep the gas pressure in the repository sufficiently low to avoid fracturing of the host rock. The aim is to increase the gas transport capacity of the backfilled underground structures without compromising the radionuclide retention capacity of the engineered barrier system. Modelling studies were carried out by Nagra (2008) to estimate the repository resaturation time, maximum pressures in the emplacement caverns and expulsion of contaminated water from the repository. The resaturation studies were carried out using a hydrodynamic site model. The assessments of the gas transport capacity of the host rock and the EBS, in order to estimate gas build-up, were carried out using TOUGH2. The most important factors controlling the various
gas pathways were identified through parametric studies. In these, the properties of the host rock, backfill and seals, along with the hydraulic and initial boundary conditions, were taken into account. The pressure build-up within the repository was found to be highly dependent on the gas storage volume of the backfill and the gas transport capacity of the host rock. The pressure build-up in the repository was estimated to be insufficient to cause fracturing of the host rock.

### 4.2.3 Recent developments

Traditionally, radionuclide migration has been considered to occur through the migration of groundwater and gases. The flow paths of gases were, however, not considered in detail until it was found that significant quantities of gas may be formed. Since then, gas migration has been identified as an area requiring further research by many countries proposing geological disposal. A European project ‘FORGE’ was established in collaboration with several waste management organisations, regulators and academia in 2010 to investigate the fate of repository gases. The project studies the impact of gas migration on the repository performance using both experimental and numerical tools. Countries participating in the project include France, UK, Spain, Czech Republic, Belgium, Germany, Switzerland, Lithuania, Finland, Romania and Sweden. The member countries’ current state of knowledge regarding gas migration has been reported in, for example, Norris (2010) and Wendling (2010).

Elsewhere, Ontario Power Generation have also performed gas migration studies for the proposed L/ILW disposal facility at the Bruce Site in Ontario, Canada. In a report prepared by Calder et al. (2009), gas and groundwater transport studies are presented using results from TOUGH2. Again, a detailed repository design has been used to assess the consequences of gas generation and migration at the Bruce disposal site. The difference between the studies carried out in the UK and Switzerland and the study by Calder et al. (2009) is that in the Canadian investigation the gas generation rate was coupled with the water inflow rate. This was achieved by using TOUGH2 in conjunction with a gas generation program GGM.

### 4.2.4 Requirement for further research

In conclusion, no sensitivity studies have been carried out to date, which systematically assess the impact of different repository designs and host rock features on gas migration. Instead, the emphasis has been on proving that repository gases do not threaten
the repository concepts in fractured and clay host rocks. The repository designs in
the studies have also been very detailed instead of assessing the relative importance of
different repository features. Internationally, some work has been conducted to look
at the sensitivity of the results for different repository features. However, these studies
generally only take into account one type of repository design. Some work has also
been carried out to look at the effects of gas in different host rocks, but this work is
lacking in depth. From this it seems that a systematic sensitivity study is needed in
order for the UK to take a more proactive approach to repository gas management.

4.3 Program selection

This section discusses the selection of a suitable program for the EngD project. The
programs currently available for modelling multiphase flow in porous media are listed,
and the selection criteria are discussed. The selected program is then introduced in
more detail.

4.3.1 Comparison of programs

There are several programs available for modelling fluid flows through different media.
Some of the programs and their capabilities are listed in Table 4.1. Table 4.2 shows
a brief description of these programs and the reasons why they have or have not been
chosen for the project.

Many programs do not possess the capability to model transport of gases in the geo-
sphere, but are intended for modelling groundwater flow and transport. TOUGH2 and
FEHM appear to be the only two currently available codes for modelling gas migration
in fractured media. Of these, TOUGH2 seems to be more established and has therefore
been chosen as the primary code for this project. TOUGH2 is a program developed at
the Lawrence Berkeley National Laboratory. It models multicomponent, multiphase
fluids in 1D, 2D or 3D porous and fractured media. Its applications lie in geothermal
reservoir engineering, nuclear waste disposal, environmental assessments and unsatu-
rated and saturated zone hydrology. More information about TOUGH2 is provided
in Section 4.3.2. TOUGH2 is already widely used in radioactive gas migration and
contaminant transport studies in the nuclear industry, which indicates its usefulness
for the type of research in question.
The Finite Element Heat and Mass transfer code FEHM is a program developed to simulate non-isothermal, multiphase flow and transport through complex 3D geologic media. It was developed at Los Alamos National Laboratory and has been used to model gas and liquid flow near the Yucca Mountain waste repository. FEHM is capable of tracking the movement of multiple gas and liquid constituents that chemically react and adsorb, as well as handling the transport of solutes that partition between the liquid and gas phases according to Henry’s Law.

FEHM seems to have similar capabilities to the TOUGH family codes. Indeed, both FEHM and TOUGH2 have previously been used by the U.S. Department of Energy to model multiphase flow and transport in variably saturated media at Yucca Mountain. In an independent study, Webb (1996) compared the use of the two programs and concluded that for their project TOUGH2 was likely to offer less CPU time and more flexible geometries. Additionally, there seems to be much more information available on studies performed using TOUGH2, which supports its selection in the current research.

### 4.3.2 TOUGH2

TOUGH2 solves mass and energy balance equations that describe fluid and heat flow in general multiphase, multicomponent systems. Mass transfer is assumed to occur by advection, diffusion and hydrodynamic dispersion. Heat flows occur by conduction and

<table>
<thead>
<tr>
<th>Program</th>
<th>2D</th>
<th>3D</th>
<th>Flow in porous media</th>
<th>Flow in fractures</th>
<th>Finite element</th>
<th>Finite difference</th>
<th>Groundwater flow</th>
<th>Gas flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>DYNA3D</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>FEFLOW</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>FEHM</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>MODFLOW</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>NAMMU</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>NAPSAC</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
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<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>SUTRA</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>TOUGH2</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
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</tr>
<tr>
<td>TOUGH+</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>TOUGHREACT</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
</tr>
</tbody>
</table>

Table 4.1: Properties of the programs investigated. Ticks indicate areas covered by the program.
<table>
<thead>
<tr>
<th>Model</th>
<th>Brief description</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>DYNA3D</td>
<td>FE program for structural/continuum mechanics problems.</td>
<td>Concentrates on structural integrity, no fluid flow capabilities.</td>
</tr>
<tr>
<td>FEFLOW</td>
<td>2D/3D model for groundwater flow and transport in porous and fractured media.</td>
<td>No gas modelling capabilities.</td>
</tr>
<tr>
<td>FEHM</td>
<td>Program for modelling multiphase multicomponent flow through porous and fractured media.</td>
<td>Similar to TOUGH2 and TOUGHREACT but less well established.</td>
</tr>
<tr>
<td>MODFLOW</td>
<td>Finite difference model for 3D groundwater flow in porous media.</td>
<td>No gas modelling capabilities.</td>
</tr>
<tr>
<td>NAMMU</td>
<td>2D/3D FE model for groundwater flow and transport through porous media. Suitable for contaminant transport.</td>
<td>No gas modelling capabilities.</td>
</tr>
<tr>
<td>NAPSAC</td>
<td>FE modelling tool for 3D groundwater flow and transport in fractured rock.</td>
<td>No gas modelling capabilities.</td>
</tr>
<tr>
<td>SUTRA</td>
<td>FE model for 2D saturated or unsaturated groundwater flow with energy transport or chemically reactive single species solute transport.</td>
<td>No gas modelling capabilities.</td>
</tr>
<tr>
<td>TOUGH2</td>
<td>Program for modelling multicomponent multiphase fluids in fractured and porous media.</td>
<td>Program widely in use in the nuclear industry worldwide.</td>
</tr>
<tr>
<td>TOUGHREACT</td>
<td>Program for modelling chemically reactive non-isothermal flows of multiphase fluids in 1D, 2D or 3D porous and fractured media.</td>
<td>Model considers a variety of equilibrium chemical reactions.</td>
</tr>
</tbody>
</table>

Table 4.2: Description of different programs.
4.3. PROGRAM SELECTION

convection. Gas dissolution is described by Henry’s Law and compression by Boyle’s Law.

TOUGH2 was written in FORTRAN77 and it employs a so-called MULKOM architecture. MULKOM architecture implies that the flow and transport aspects of the problem - which do not depend on the nature and number of fluid components and phases - are separated from the fluid property and phase composition aspects, as these are specific to the particular fluid mixture. The structure of TOUGH2 is shown in Figure 4.1.

![Figure 4.1: TOUGH2 structure.](image)

An equation-of-state (EOS) module needs to be added to the core program. These modules provide the thermo-physical properties of fluid mixtures needed for assembling the mass and energy-balance equations. The EOS modules useful for this project are:

- EOS3 (water, air) - e.g. initial resaturation of the repository
- EOS5 (water, hydrogen) - e.g. corrosive metals placed in the repository
- EOS7R (water, brine, radionuclide 1, radionuclide 2, air) - e.g. radionuclide migration

The following sections describe the use of TOUGH2, the assignment of boundary conditions and the way TOUGH2 can handle fluid flow through fractures. These concepts
will be used in the numerical modelling studies presented in the later chapters.

### 4.3.2.1 Use of TOUGH2

TOUGH2 is available for purchase from Lawrence Berkeley National Laboratory. For this project, however, TOUGH2 was obtained free of charge through the NEA data-bank. This service is offered to scientists in the NEA member countries, with the aim of collectively developing tools commonly used in the nuclear industry.

The author initially attended a 3-day course at the Lawrence Berkeley National Laboratory to be trained to use TOUGH2. Several months were then spent running test examples and setting up the mesh generation and data processing systems. During this time the use of different applications was investigated and PetraSim was selected as a pre and post-processor for TOUGH2. It was found that PetraSim provides an easy-to-use graphical interface for preparing input files and examining initial results. PetraSim has TOUGH2 built in, so that the mesh generation, running of the models and data processing can all be handled within the program. A 1-day course on the use of PetraSim was also attended whilst at Lawrence Berkeley. After initial trial runs it was found that the pre and post processing capabilities of PetraSim were inadequate for the scope of the investigations to be performed. It was kept for mesh generation purposes, but MATLAB was utilised to edit the TOUGH2 input files and to read and analyse the data generated from the runs. This allowed automation of the investigations to be achieved and large batch runs to be performed.

TOUGH2 runs on a normal PC with minimal memory requirements. The sizes of the input and output files are dependent upon two factors: the number of elements in the mesh and the number of timesteps at which a printed output is produced. Both of these parameters can be modified by the user. In PetraSim, the maximum number of elements is set to 50,000, while the maximum number of elements in TOUGH2 itself can be varied in the source file. The input and output files are in a text file format, the sizes of which ranged from few megabytes to several dozen gigabytes for the largest models. In this project one PC was used continually, and another one was utilised when large batch runs were required.

The TOUGH2 run times varied from few seconds to several days. For most cases presented in Chapters 6 - 8, the run times were between 3 and 6 hours. The processing of the results was found to take almost as long as the running of the program itself. It was, therefore, important to decide before hand what output was required in each case,
to reduce the required computational time and hard disk space. Note on TOUGH2 output: The TOUGH2 output data varies depending on the number of phases present in each element. If only water is present, the pressure data expresses the pore water pressure. If both gas and water are present, the pressure data refers to the pore gas pressure. This thesis considers almost entirely multiphase systems and, where the term pore pressure is used, this should be taken to refer to the pore gas pressure.

TOUGH2 is well established as a multiphase flow simulator and many studies have looked at the accuracy of the TOUGH2 results in comparison with experimental or analytical results (see TOUGH2 User Guide for further information: Pruess et al., 1999). It also allows certain simplifications to be made by, for example, utilising automatic timestepping instead of using fixed timesteps throughout the runs. This eases the running of cases with very long timescales. The program is not, however, very user-friendly, and difficulties were encountered on several occasions. For example, the output files of TOUGH2 and PetraSim vary in format, different types of data (for example pressure and flow data) use different formatting within the same file, the numbering in TOUGH2 is not consistent (zeros in numbers are not written out, so that number 11015 is written as 11 15), etc. Additionally, PetraSim fell short of what would be required of a modern mesh generator and many errors in the code meant that on occasion some output data was lost and had to be re-run using the standalone TOUGH2 solver.

As an example of mesh generation problems in PetraSim, only horizontal planes of elements can be examined within a model, whilst vertical planes are not shown, and the simultaneous selection of multiple elements is made difficult. This meant that, for example, assigning initial conditions for 50,000 elements was very time-consuming, as each element had to be selected individually. Additionally, input files produced in PetraSim cannot be manually modified and re-run, which confirmed the need for MATLAB as a data processing tool. In hindsight, the time spent learning to use PetraSim would have been better spent developing a more flexible meshing tool.

4.3.2.2 Boundary conditions in TOUGH2

Constant thermodynamic boundary conditions (i.e. Dirichlet boundary conditions), can be achieved in TOUGH2 using either large volume or inactive boundary elements. In the case of large volume elements, the grid blocks adjacent to the boundary are assigned very large volumes of the order of $10^{50}$ m$^3$. Any fluid or heat exchange with
the rest of the system will then not change the thermodynamic conditions in the large-volume elements significantly enough to be able to affect the conditions in the neighbouring elements. Time-dependent thermodynamic conditions can be achieved by specifying a sink/source in the large volume element. Alternatively, inactive elements offer a way to set up boundary conditions and to shorten computational time. The thermodynamic conditions of the inactive elements remain unchanged throughout the simulation, as mass and energy balances do not need to be calculated for these elements.

Fluxes of mass or heat across the boundary (i.e. Neumann boundary conditions) can be specified by introducing a sink/source into the element adjacent to the boundary. The conditions can therefore easily be made either constant or time-dependent. A special case of Neumann conditions is when there is no flux across the boundary. This is the default setting in TOUGH2.

4.3.2.3 Fracture flow in TOUGH2

TOUGH2 provides a way of modelling fluid flow in fractured media called ‘Multiple INteracting Continua’ (MINC). The MINC concept is based on the idea that fractures have large permeabilities and small porosities and, as such, any changes in reservoir conditions, such as temperature or pressure, will penetrate quickly through the fracture network. The rock matrix has opposite characteristics and any changes will penetrate the rock matrix slowly. Therefore, global flow only occurs through the fractures.

Figure 4.2 shows the classical double porosity concept where low permeable matrix blocks are surrounded by a network of fractures. Global flow occurs through the fractures only, but the matrix and fractures can exchange fluid and heat through interporosity flow driven by pressure and temperature differences.

The MINC concept takes this idea a step further, in order to account for multiphase and non-isothermal flow systems where interporosity flow can be very slow. Here the matrix conditions are controlled by the distance from the fractures. In TOUGH2, a mesh is first created as usual and this is then processed to generate a secondary mesh which carries all information required to describe interporosity flow. Each gridblock is discretised into small nested volumes as shown in Figure 4.3.

As the fractures form an interconnected network, all fractures can be considered to form a continuum with uniform conditions. Similarly all material within a certain distance from the fractures is lumped into a second continuum, all material within a slightly
larger distance into a third continuum, and so on. The secondary mesh is created using user-specified volume fractions of the fracture and matrix material, and a proximity function. A proximity function expresses the total fraction of matrix material within a distance $x$ from the fractures for a given domain $V_0$. The MINC process then calculates the volumes, interface areas and nodal distances for the new mesh. Enabling global flow in the matrix is possible in MINC. However, it should be remembered that MINC can only be applied to situations where fractures are considered to form a continuous network.

In some multiphase flow problems the fluid phases have very different flow properties. An example of such a case is the flow of air and water in a fractured unsaturated medium. Capillary forces allow the flow of the non-wetting phase primarily through the fractures, while the wetting phase flows through the matrix. Systems like this exhibit ‘dual permeability’ characteristics. MINC can be generalised to include global matrix-matrix flow connections, and modelling global flow through the matrix is thus possible. Pruess (1992), however, warns that great care must be taken to avoid unphysical behaviour. (Note - Unphysical behaviour here refers to something that would not happen in the nature but is introduced to the model due to numerical approximations. It can often be avoided through parameter choices.)


4.4 Discussion

This chapter further refined the problem that this EngD aims to solve through numerical modelling. Previous studies in the field were summarised, and it was found that no studies have been performed to date which compare the effects of different repository features on gas migration. TOUGH2 was identified as the most suitable program for use in the project, as it is one of the few programs available for modelling multiphase flow and already widely used within the nuclear industry.

The next chapters, comprising the main body of the EngD thesis, concentrate on demonstrating the behaviour of repository gases in the underground environment. TOUGH2 is used, first, to improve understanding of the processes taking place in the repository, and then to carry out a parametric study which compares the repository design and layout options. Finally, gas transport through the host rock is also modelled using TOUGH2. These studies examine the effects of the repository features on the gas migration, with the ultimate aim of improving the safety of the repository with regard to gas generation and migration.
Chapter 5

Behaviour of Repository Gas

This chapter investigates the basic processes taking place in a pressurised gas-water system using the results of a series of simple TOUGH2 simulations. The aim of these experiments is to improve understanding of the behaviour of repository gases and the use of TOUGH2 and PetraSim.

Most calculations presented in this chapter involve the use of simple 2D models. These models are used to investigate what happens to air and gas produced within the repository after its closure. The chapter is divided into three main sections. The first section considers the resaturation phase, during which groundwater slowly fills the facility. The second section describes how gas accumulates within the repository, dissolves and migrates out into the host rock. The final section examines the flow of gas outside the repository. The experiments demonstrate qualitatively what is expected to happen to the gases, while also exploring some of the capabilities of TOUGH2 and making recommendations for its use in further work.

5.1 Resaturation investigations

After backfilling of the vaults and tunnels, the pore space within the repository structures is initially at atmospheric pressure and mostly filled with air. Water from the surrounding host rock will then start to penetrate the repository. This section considers simple cases of water flow into an air-filled porous medium. The behaviour of air initially trapped within the repository is described using results from TOUGH2 simulations.
5.1.1 Resaturation model description

Figure 5.1 shows the set-up of the resaturation problem. The initial conditions are indicated in the part (a) of the figure, while the boundary conditions are shown in part (b). An area of $10 \, m \times 1 \, m \times 30 \, m$ was selected, and it was divided into 300 elements, each with dimensions of $1 \, m \times 1 \, m \times 1 \, m$. The top and side boundaries were assumed to be impermeable. Constant pore pressure and gas saturation were held at the bottom boundary. The bottom elements also provided an infinite source of water and a sink for gas due to the use of artificially introduced very large volume grid blocks as the boundary conditions at the bottom (see discussion in Section 4.3.2.2).

Figure 5.1: The resaturation problem. The repository (in light brown) overlies an area of host rock (in blue). Water flow from the host rock into the initially air-filled repository is simulated. Image (a) shows the model set-up and initial conditions, while (b) shows the boundary conditions that were applied.

The pore pressure in the host rock was set to 3 MPa, corresponding to the hydrostatic pressure at a depth of approximately 300 m, and the host rock was assumed to have an initial air-saturation of 0.001. The repository was initially at atmospheric pressure and had an air saturation of 0.90. The movement of water and gas between the backfill and host rock were simulated.
The resaturation investigations considered the rate of groundwater flow into the repository and the behaviour of air within it. These two-phase calculations are strongly affected by the permeabilities of the materials and the relative permeability and capillary pressure curves. The hydrogeological properties used in the resaturation calculations are presented in Table 5.1.

<table>
<thead>
<tr>
<th></th>
<th>Host rock</th>
<th>Backfilled repository</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability (m²)</td>
<td>$1.0 \times 10^{-16}$</td>
<td>$6.1 \times 10^{-17}$</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.15</td>
<td>0.08</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>$S_{LR}$</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$S_{GR}$</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>$P_0$ (Pa)</td>
<td>$2.0 \times 10^6$</td>
<td>$2.0 \times 10^6$</td>
</tr>
</tbody>
</table>

Table 5.1: Material and two-phase flow parameters for the base case resaturation investigations.

The relative permeability and capillary pressure functions by van Genuchten (1980) were used. The parameters required to define these curves were chosen as below.

- Adjustable parameter related to the pore size distribution, $\lambda$. Several authors suggest that $\lambda = 0.5$ would be a typical value for porous media (see for example the discussion in Bate et al., 2007).

- Irreducible liquid saturation, $S_{LR}$. For this study, $S_{LR} = 0.3$ was used, as this seemed to be a common value in previous studies, such as Bate et al. (2007) and Senger et al. (2009).

- Irreducible gas saturation, $S_{GR}$. A small $S_{GR}$ implies that the gas phase becomes mobile at small saturations. The value $S_{GR} = 0.003$ was used in line with studies by Nagra (2008) and Senger et al. (2009).

- Gas entry pressure, $P_0$. Value $P_0 = 2.0 \times 10^6$ Pa was used as this was close to the values selected by Bate et al. (2007), Nagra (2008) and Senger et al. (2009).

The permeability of the host rock was chosen to be $k = 1.0 \times 10^{-16}$ m², as may be the case for a fractured rock. The repository materials are assumed to be homogeneous and to have the combined properties of the waste packages and backfill. The permeability of the repository is chosen to be $k = 6.1 \times 10^{-17}$ m², in line with the study by Bate et al. (2007). A small porosity value, as used by Hoch and Swift (2010), is used in
order to describe pressure build-up within the pores in the repository.

Gravity was ignored initially, but variations of the base case were carried out to look at its effect on the results. The effect of the repository depth and the permeability of repository materials and the host rock were also studied. Temperature changes were not taken into account in any of the investigations presented in this thesis due to the non-heat producing nature of L/ILW.

### 5.1.2 Resaturation results

This section aims to demonstrate the behaviour of air trapped in the repository during the resaturation phase using results from the TOUGH2 simulations. PetraSim was used to construct the meshes and to look at the initial results. MATLAB was also used as a data processing tool.

![Graph](image)

Figure 5.2: The rate of groundwater flow from the host rock into the repository after the repository has been closed.

It was found that groundwater enters the repository almost instantaneously. Due to the large pressure gradient between the host rock and the repository, water starts to flow into the repository rapidly. Figure 5.2 shows the flow rate of water across the interface between the host rock and the repository. It can be seen that the inflow rate
Figure 5.3: Pressure drawdown area. The pore pressure is initially atmospheric in the repository and 3 MPa in the host rock. The images show how the pore pressure in the host rock decreases temporarily as water flows into the repository. Over time, water from the host rock, below the area shown here, fills the system and the pore pressure tends towards 3 MPa.
of water reduces over time as the pressure gradient between the pores of the host rock and the repository reduces.

The groundwater flow into the repository affects the pore pressure in the host rock: the pressure reduces and a pressure drawdown area is formed. Figure 5.3 shows how the pore pressure decreases in the elements below the repository. It can be seen that four weeks after the start of the simulation the pore pressure in the host rock is noticeably lower than it is at the start of the simulation. This pressure drawdown extends to all the elements below the repository. Figure 5.4 shows the pore pressure changes in an element at the bottom of the system. The pressure decrease is felt in this element after only a couple of hours. Slightly over a year later, the pore pressure returns to the initial level. The overshoot in the pressure is due to the fact that gas pressure is shown instead of the water pressure. The increase over 3 MPa is therefore due to the capillary pressure experienced in areas which contain air in gaseous form. Over time, pore pressure reduces slowly, as dissolved air is transported away from the site of dissolution and more air can dissolve. After a very long period of time, the gas pressure would approach the initial pore pressure of the host rock, 3 MPa.

Figure 5.4: Pore pressure changes at the bottom of the system. The image shows how the pressure drawdown is felt at the bottom of the system. The pore pressure there decreases temporarily, but over time returns to values greater than 3 MPa.

Figure 5.5 shows the pore pressure, gas saturation and mass fraction of dissolved air in Element P (see Figure 5.1) in the centre of the repository over time. The pore pressure
starts off at atmospheric, and the gas saturation at 0.9. One year after the start of the simulation, the pore pressure in Element P starts to slowly increase, as the air is compressed due to water breaking into the repository. Between years two and three, the water front reaches Element P and the pore pressure increases to values over 3 MPa. The pressure increase results in the rapid dissolution of most of the air. Over time, gas saturation and pore pressure in Element P reduce slowly, as dissolved air is transported away from the site of dissolution and more air dissolves. After several thousand years, the gas pressure approaches the initial pressure of the host rock, 3 MPa, and the gas saturation approaches 0.001. The mass fraction of dissolved air starts at a very small value which corresponds to the solubility of air at atmospheric pressure. As the pore pressure increases, more air can dissolve, and so the shape of the curve follows closely that of the pore pressure curve.

Figure 5.5: Pore pressure, gas saturation and mass fraction of dissolved air in Element P over time. The figures show how the increasing pore pressure allows air to dissolve between years two and three.

Henry’s Law states that the partial pressure of a gas in the gaseous phase is proportional to the mole fraction of dissolved gas in the aqueous phase (see Chapter 3). Pruess et al. (1999) take Henry’s constant to be $6.7 \times 10^9$ Pa. The amount of dissolved air initially in the system when the air pressure is atmospheric, and after 10,000 years, can
be estimated using the pore pressure curve in Figure 5.5. The values obtained from this calculation are close to those shown in the mass fraction curve in Figure 5.5, and differ by 4% initially, and by 7% after 10,000 years.

As the water front advances upwards towards the top of the repository, the air is pushed to the top in front of it. The space within which the air is contained reduces and the air compresses. Figure 5.6 shows the density of air in Element P. The density increases rapidly between the years two and three, which is when the groundwater front reaches the element.

![Figure 5.6: Density of air in Element P. The groundwater front reaches the element between the years two and three and compresses air.](image)

According to Boyle’s Law, the air pressure, $P$, and volume, $V$, are inversely proportional, i.e.

$$P_1 V_1 = P_2 V_2$$  \hspace{1cm} (5.1)

Thus

$$\frac{\rho_2}{\rho_1} = \frac{P_2}{P_1}$$  \hspace{1cm} (5.2)

The initial pore pressure of the air is known, and the final pore pressure can be obtained from from Figure 5.5. The initial gas density, $\rho$, can be obtained from Figure 5.6. The final gas density can therefore be calculated and compared with the value.
in Figure 5.6. The calculated value is found to differ by less than 3% of the value obtained from TOUGH2.

Figure 5.7: Demonstration of the pore pressure and gas saturation profiles at different times. The red line indicates the boundary between the repository and the host rock. The atmospheric pressure and initial saturation of 0.9 are also indicated. Over time, the pore pressure in the system tends towards, and exceeds, 3 MPa. The gas saturation reduces, as air dissolves and spreads throughout the entire system.

Figure 5.7 summarises the behaviour of the system by showing snapshots of the pore pressure and gas saturation profiles at different times. Shortly after closure, the pore pressure is atmospheric in the repository and hydrostatic in the host rock. The gas saturation is 0.9 in the repository and 0.001 in the host rock. As time goes by, the pore pressure in the repository increases as water flows in. Any changes in pore pressure propagate through the air-filled area fast, so that constant pore pressure is maintained in these areas. Gas saturation is still 0.9 in the upper parts of the repository, but less in areas which have been partly or fully filled with water. Almost all the air has dissolved in the lower parts of the repository which are now fully saturated. The pressure drawdown area causes pore pressure to be linearly increased from 3 MPa at the bottom to the pore pressure which the air at the top of the repository experiences. The slight skewing of the line is due to the capillary pressure effects in areas with
gaseous air. Ten years after the start of the simulation, the pore pressure has reached 3 MPa throughout, indicating that the system is now fully saturated. In areas where some air still remains in gaseous phase, the gas pressure reaches values over 3 MPa. Over thousands of years, gas diffuses into the entire system and pore pressure and gas saturation become uniform throughout.

The timing of the changes shown in Figures 5.5 and 5.7 is heavily dependent on the permeability of the materials and the driving pressure, and hence the depth of the repository. The effect of these parameters on the results was investigated next.

![Figure 5.8: The effect of the repository permeability on gas migration. The higher the repository permeability is, the faster the water front travels through the repository. The pore pressure in the repository thus increases, and the gas saturation decreases, faster for the higher permeability cases.](image)

First, the permeability of the repository material was changed to values higher and lower than in the original case. The permeability of the host rock was kept constant at $1.0 \times 10^{-16} \text{ m}^2$. The repository material of higher permeability was given a value of $6.1 \times 10^{-15} \text{ m}^2$, i.e. it was more permeable than the host rock. The material in the second case was given a permeability one order of magnitude lower than the original case, i.e. $6.1 \times 10^{-18} \text{ m}^2$. The results are shown in Figure 5.8. In the higher permeability case, the water front penetrates the repository at the same time as in the original case, but travels through the repository faster. It reaches the top of the repository before
Figure 5.9: The effect of the initial pore pressure of the host rock on gas migration. The higher the initial pore pressure is, i.e. the deeper the repository is located, the faster the groundwater flows into and through the repository.

1 year and most of the air dissolves. The faster flow into the repository also affects the extent of the drawdown area in the host rock; the pore pressure in the host rock is reduced more than in the original case. In the lower permeability case, water again breaks through at the same time, but travels through the repository at a much slower rate. The pore pressure in the surrounding host rock returns to normal quicker than in the other two cases. The pore pressure and gas saturation curves look much like those detected at earlier times using the original value for permeability, as shown in Figure 5.7.

The effect of the repository depth was investigated next. This affects the initial pore pressure of the host rock, and thus the driving pressure gradient. Figure 5.9 compares the gas saturation profiles of the repository excavated at a depth of approximately 100 m, 300 m and 500 m after 100 years. It can be seen that the gas saturation is the largest in the case with the smallest driving pressure, 1 MPa, as the water front penetrates the system at a lower rate, and dissolution of gas occurs later. Similarly, the highest initial pore pressure, 5 MPa, causes groundwater to flow into and through the repository at a faster rate. This gives time for the dissolved gas to be transported downwards in the column, and thus the gas saturation in the top parts of the repository is lower compared to the other two cases.

A small-scale sensitivity experiment was conducted to investigate the sensitivity of the
Figure 5.10: The sensitivity of the resaturation time to the permeability of the repository. A linear dependence between the resaturation time and the permeability of the repository is detected.

\[ y = -2.46 \times 10^7 x + 7.89 \times 10^7 \]

Figure 5.11: The sensitivity of the resaturation time to the pore pressure of the host rock. A linear dependence between the resaturation time and the pore pressure of the host rock, i.e. the depth of the repository, is detected.

\[ y = -24.6 x + 1.7 \times 10^8 \]
5.1. RESATURATION INVESTIGATIONS

<table>
<thead>
<tr>
<th>Permeability of the repository ($\times 10^{-17} \text{m}^2$)</th>
<th>Pore pressure in the host rock (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case</td>
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</tr>
<tr>
<td>Variant 1</td>
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<tr>
<td>Variant 2</td>
<td>5.90</td>
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<td>Variant 3</td>
<td>6.20</td>
</tr>
<tr>
<td>Variant 4</td>
<td>5.80</td>
</tr>
<tr>
<td>Variant 5</td>
<td>6.00</td>
</tr>
<tr>
<td>Variant 6</td>
<td>6.00</td>
</tr>
<tr>
<td>Variant 7</td>
<td>6.00</td>
</tr>
<tr>
<td>Variant 8</td>
<td>6.00</td>
</tr>
</tbody>
</table>

Table 5.2: Sensitivity experiment.

resaturation time to the changes in the permeability and the repository depth. All parameters except the permeability of the repository and the pore pressure of the host rock were kept constant. The cases are presented in Table 5.2. The time for Element P to reach full saturation was recorded in each case, and the dependence of the saturation time on either the permeability of the repository or the pore pressure of the host rock was investigated. The element was assumed to be saturated when it contained 0.9 water. The results are shown in Figures 5.10 and 5.11.

Figure 5.10 shows that there is a linear dependence between the resaturation time and permeability. It can be seen that a $0.1 \times 10^{-17} \text{m}^2$ change in permeability results in the change of approximately 3 days in the resaturation time. This indicates that the resaturation time can be affected by a couple of years by selecting materials with optimum properties. This information could be used when determining, for example, the timing of backfilling of different vaults.

Another way of dealing with uncertainties would be to use a statistical approach and to allocate each element a permeability randomly based on the probability of different permeabilities existing in certain types of media. A large number of different combinations of permeabilities could be created using a random field generator, and the results of the runs with the different material data could be compared. This, however, requires far more computational effort than the sensitivity study presented above.

Figure 5.11 shows that there is a linear dependence between the resaturation time and the pore pressure of the host rock, i.e. the depth of the repository. It can also be seen that a 0.1 MPa change in pore pressure results in the change of approximately 30 days in the resaturation time. This indicates that if the repository was placed several hundred metres deeper, the resaturation would occur a couple of years sooner.
The effect of gravity was also investigated, as it was ignored in the original case. Figure 5.12 shows the pore pressure profiles of the system at 1 year and 100 years after the start of the simulation with and without gravity. Gravity slows down the water front, and results in slightly smaller pore pressures in the upper regions. This effect is, however, almost unnoticeable at early times. Gravity should be taken into account when looking at areas with large vertical extent relative to the repository depth, or long timescales. The effect of gravity on horizontal flows is investigated in the following section.
5.2 Near field investigations

The inflowing groundwater will start gas generation processes within the repository. Large quantities of hydrogen gas will be produced primarily as a result of corrosion. The gas will initially accumulate within the repository structures. When the gas pressure in the repository rises to a level high enough to overcome the capillary entry pressure of the host rock, gas may migrate out of the repository. Dissolved gas is removed with the groundwater. If the removal rate of hydrogen is less than the generation rate, the pore pressure in the repository increases. In some rocks of low permeability, such as clays, the capillary entry pressure may be very large. This may cause the pore pressure to rise to levels high enough to cause damage to the repository structures.

5.2.1 Vertical model description

This part of the study investigates the pore pressure increase in the repository and the two-phase flow of hydrogen out of the repository using the set up shown in Figure 5.13. The repository area is now located between two areas of host rock with a permeability of \( k = 1.0 \times 10^{-16} \text{m}^2 \), so that gas flow upwards, as well as downwards, is allowed. Gravity is now enabled and hydrostatic conditions are applied throughout the system, with the average pore pressure set to 3 MPa. In order to investigate the removal rate of hydrogen, the gas saturation of the repository is initially set to 0.5, and there is a small amount of hydrogen, 0.0001, initially present in the host rock. Gas is expected to move primarily upwards due to buoyancy forces.

The pressure build-up problem involved investigating an area of 10 m × 1 m × 45 m, with an element size of 1 m × 1 m × 1 m. The side boundaries were set to be impermeable, and both the top and bottom were assigned constant hydrostatic pressure conditions. The top and bottom boundaries again represent large volumes of host rock which provide an infinite supply of groundwater and a sink for gas. The same material and two-phase flow parameters as in the previous section were used (see Table 5.1). Gravity was taken into account in order to maintain hydrostatic pressure.

The system described above was used to investigate the potential pore pressure increase within the repository and the way hydrogen migrates out of the repository. Variations of the base case involved using a constant gas generation rate instead of an initial gas saturation within the repository.
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Figure 5.13: The vertical pressure buildup problem. The repository (in light brown) is located between two areas of host rock (in blue).

5.2.2 Vertical model results

Figure 5.14 shows the pore pressure and gas saturation profiles of the system at different times. Hydrostatic pressure has been subtracted so that the results can be compared with Figure 5.7. As water flows into the repository, the pore pressure there increases and some of the hydrogen dissolves. At the same time, gas is able to migrate both upwards and downwards into the host rock, although its movement upwards is quicker due to buoyancy forces. This results in the pore pressure profiles being asymmetric about the centreline. After 10 years, gas in both gaseous and liquid phases can be detected everywhere in the system. The pore pressure in the repository stays below 4.2 MPa at all times. Figure 5.15 shows the changes in pore pressure, gas saturation and fraction of dissolved hydrogen gas in Element Q in the middle of the repository. Initially, the pore pressure is 3 MPa throughout and the gas saturation is 0.5 in the repository. The rate of water flow into the repository is initially high (see Figure 5.16), but reduces over time. The pore pressure in the repository increases as groundwater flows in, and this increases the mass fraction of dissolved gas in the element. A continuous gas pathway from the repository into the top and bottom row elements becomes established after approximately 2 years. This speeds up the removal rate of hydrogen, and so the pore pressure in the repository gradually starts to reduce.

For the above calculation, an initial gas saturation was required. This was then changed to a constant gas production rate to achieve a more realistic situation. Hoch and Swift
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Figure 5.14: Demonstration of the pore pressure and gas saturation profiles at different times for the system shown in Figure 5.13. As water flows into the repository, the pore pressure there increases and some of the hydrogen dissolves. At the same time, gas is able to migrate both upwards and downwards into the host rock.

Figure 5.15: Pore pressure, gas saturation and mass fraction of dissolved hydrogen in Element Q over time. As the pore pressure in the element increases, hydrogen dissolves. Over time, dissolved hydrogen spreads throughout the entire system and the fraction of dissolved hydrogen in Element Q reduces.
Figure 5.16: The rate of water flow across the top boundary of the repository. The rate of water flow into the repository is initially high, but reduces over time.

Figure 5.17: Pore pressure and gas saturation in Element Q over time with steady state hydrogen production in the repository. The pore pressure in the middle of the repository starts to increase early and reaches a maximum value of approximately three times the hydrostatic pressure. A continuous gas pathway between the repository and the elements at the top becomes established after approximately 4 months, which results in a more efficient removal of gas and a decrease in pore pressure. After 11 years, a steady state is reached and gas is removed at the same rate as it is produced.
(2010) estimated the gas generation rates in different environments using the UK waste inventory. Their calculations showed that the steady state gas generation rate in fractured rock, salt and clay is approximately 1000 m$^3$/year. This amount was distributed evenly between the elements making up the repository, i.e., 150 elements, and corresponds to the generation rate of $2 \times 10^{-8}$ kg/s per element.

Figure 5.17 shows the results of the run with the steady state production rate. The pore pressure in the middle of the repository starts to increase within hours, and reaches a maximum value which is approximately three times the hydrostatic pressure. The maximum pore pressure is reached approximately 4 months after the start of the hydrogen production. This is when a continuous gas pathway between the repository and the elements at the top becomes established and gas starts to be removed more efficiently. After this, the pore pressure in the repository reduces until approximately 11 years. The gas saturation in the repository starts to build up after a month, and increases steadily until about 11 years. After 11 years, a steady state is reached and gas is removed at the same rate as it is produced. The pore pressure and gas saturation therefore stay constant at approximately $P = 5.6$ MPa and $S_g = 0.28$. This scenario is not realistic in the sense that the repository volume here is very small compared to the actual one. In the actual case, the pore pressure and the gas saturation in the repository would be expected to remain much lower.
5.2.3 Horizontal model description

The system described in Section 5.2.1 was then turned sideways, as shown in Figure 5.18, to investigate the effect of a regional groundwater flow. Hydrostatic pressure was applied in the vertical direction, and a pressure gradient in the horizontal direction. This induced a horizontal groundwater flow regime which was expected to transport the gas from the repository outwards towards the right hand side of the system. The top and bottom boundaries were assumed to be impermeable, and constant pore pressure and gas saturation were held on the sides of model which represented large areas of host rock. The average pore pressure of the system was set to 3 MPa throughout, but an additional 0.1 MPa was added to all the elements on the left hand side to drive horizontal flow through the repository. This corresponds to a hydraulic gradient of 0.22.

\[ P = \text{hydrostatic} + 0.1 \text{ MPa} \]

\[ P = \text{hydrostatic} \]

\[ S_g (\text{H}_2) = 0.5 \]

Figure 5.18: The horizontal pressure buildup problem. The repository (in light brown) is located between two areas of host rock (in blue).

The above study was also carried out using a 45 m × 10 m × 10 m 3D model. This was done to ensure that the results would be consistent with the 2D case. Constant pore pressure and gas saturation boundary conditions were applied to all the elements on the y-z plane. These sides of the model once again represented large volumes of host rock with infinite quantities of groundwater and a very small gas saturation of 0.0001. Zero-flow Dirichlet boundary conditions prevailed on the boundaries on the z-x and x-y planes.

5.2.4 Horizontal model results

The migration of gas in the horizontal system is demonstrated in Figure 5.19. At the start of the simulation, the gas saturation is 0.5 in the repository and 0.0001 in the host
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rock. The gas then starts to migrate out of the repository and water moves in. Most of the gas dissolves. Over time, the horizontal groundwater flow and the buoyancy forces push the remaining gaseous hydrogen towards the top right corner of the system. The maximum gas saturation is now much lower than the initial 0.5 indicating that most of the gas has dissolved or left the system.

The results of the 3D model of the horizontal system are shown in Figure 5.20. The results were found to be very similar in the 2D and 3D calculations, but the gas migrated out of the repository slightly quicker in the 3D case. This is due to the slightly different boundary conditions imposed. Figure 5.21 shows a plan view of the system at 1 year. The gas from the repository can be seen to migrate outwards in both directions, but more gas migrates to the right due to the imposed groundwater flow in this direction.
Figure 5.19: Gas saturation - evolution in 2D. The gas saturation in the repository is initially 0.5. As water enters the repository, most of the gas dissolves. The remaining gas migrates towards the top right corner of the system due to the horizontal pressure gradient and buoyancy.
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(a) 1 second
(b) 1 year
(c) 10 years
(d) 2000 years

Figure 5.20: Gas saturation - evolution in 3D.
Figure 5.21: Vectors of gas flow at 1 year. The plan view of the repository is shown. Gas can be seen to leave the repository in both directions, but more gas migrates to the right with the groundwater flow.
5.3 Far field investigations

This section considers the transport of water and hydrogen in the far field, which here means the initially fully saturated geological medium. Calculations showing the flow of fluids in media with different hydrogeological properties are provided, and investigations into the effects of rock features are carried out. Particular attention is paid to formations of low permeability, which will act as barriers to flow, and the presence of faults, which may provide a preferential pathway to the repository gas.

Water or air was injected into an injection element in an infinite line of point sources, as shown in Figure 5.22. Due to symmetry, only one of the sources and an area of \(105 \text{ m} \times 900 \text{ m}\) around it needed to be considered. This was divided into 420 elements, each sized \(15 \text{ m} \times 15 \text{ m}\). The model had a depth of 1 m. No flow boundary conditions were used on both sides of the model, whilst pore pressure and gas saturation were kept constant at the top and bottom. The top and bottom elements represented infinitely large areas of host rock so that gas flow out of the model and water flow into and out of the model were allowed. The pore pressures at the top and bottom were assumed to be atmospheric and 8.8 MPa (i.e. hydrostatic pressure at the depth of 900 m) respectively.

The host rock was assumed to be initially fully saturated with a hydrostatic pressure profile. A point source was placed into an element at a depth of 700 m. The sections below initially describe the flow of water through the rock column and then repeat the experiments using gas instead of water. In the final stage, the effect of different rock features on the transport of water and gas is investigated. These features are shown in Figure 5.23 and include:

- a low permeability host rock underlying a high permeability rock;
- a low permeability ‘capping’ barrier rock directly above the injection source and
- a high permeability fault.

The elements were assigned different rock properties so that the effect of the above-mentioned rock formations could be studied. Additionally, the grid was refined for some of the simulations. The initial and boundary conditions in these cases were the same as those described above, unless otherwise stated in the problem description.

The injection rate in all the cases considered was \(1.0 \times 10^{-6} \text{ kg/s}\). The flow through high and low permeability host rocks was investigated. Corey’s relative permeability curve was used in all the far field investigations, while, for simplicity, the capillary pressure effects were ignored. The rock and two-phase flow properties are shown in
Figure 5.22: Far field investigations. A source of water/gas in an infinite line of sources and the rock column above and below the source were considered.

Figure 5.23: The effects of high and low permeability rock formations on gas flow were investigated. The investigations included cases in which a high permeability layer overlies a low permeability layer, cases which consider the effect of non-linear ‘capping’ barriers above the injection source and cases which study the effects of higher permeability ‘faults’.
Table 5.3.

<table>
<thead>
<tr>
<th></th>
<th>High permeability host rock</th>
<th>Low permeability host rock</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability (m²)</td>
<td>$1.0 \times 10^{-17}$</td>
<td>$1.0 \times 10^{-20}$</td>
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<td>0.10</td>
</tr>
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<td>$S_{LR}$</td>
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<td>0.3</td>
</tr>
<tr>
<td>$S_{GR}$</td>
<td>0.05</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 5.3: Material and two-phase flow parameters for the base case far field investigations.

5.3.1 Single phase flow in a porous medium

5.3.1.1 Problem description

The first part of the far field problem involved investigating the flow of water through a homogeneous column of rock with a very low permeability of $k = 1.0 \times 10^{-20}$ m². Water was injected into the injection element at a rate of $1.0 \times 10^{-6}$ kg/s. This corresponds to an annual water injection rate of 30 m³. A higher permeability of $1.0 \times 10^{-17}$ m² was used to investigate water flow in a more permeable environment. The use of different boundary conditions was also studied.

5.3.1.2 Results

Figure 5.24 shows the pore pressure variation with depth along the centre of the low permeability rock column, when water is injected into an element at a depth of 700 m. Hydrostatic pressure has been subtracted so that only the pore pressure increase due to injection, and its variation with depth, is shown. It can be seen that the pore pressure is largest close to the injection element and reduces with distance. One year after the injection starts, pore pressure has increased in elements less than 30 m away from the source. Over time water penetrates further into the system, so that pore pressure there increases as well. After 1,000 years, the pore pressure increase is felt in elements over 300 m away from the source, and the maximum pore pressure is approximately one order of magnitude higher than the hydrostatic pressure.

The permeability of the host rock was then increased from $1.0 \times 10^{-20}$ m² to $1.0 \times$
Figure 5.24: Pore pressure profiles at different times for the single phase flow in an environment with low permeability. The pressure profiles along the centreline of the model are shown. The pore pressure increases in the injection element and areas above and below it.

$10^{-17} \text{ m}^2$, in order to increase the flow rate away from the injection element. The injected water now penetrates into the entire rock column as shown in Figure 5.25. After 100 years almost steady state conditions have been achieved. The pressure gradient from the injection element upwards is almost constant at $-170 \text{ Pa/m}$ (see Figure 5.25), and so the water flux through the elements is constant. We can now calculate the expected water flux using Darcy’s Law. The viscosity of water at $25^\circ \text{C}$ temperature is given in Holland and Bragg (1995, p. 48) and taken to be $1.0 \times 10^{-3} \text{ Pa} \cdot \text{s}$.

$$
F = -k \frac{\rho}{\mu} (\nabla P)
$$

$$
= -1.0 \times 10^{-17} \text{ m}^2 \frac{1000 \text{ kg/m}^3}{1 \times 10^{-3} \text{ Pa} \cdot \text{s}} \times (-170 \text{ Pa/m})
$$

$$
= 1.7 \times 10^{-9} \text{ kg/(m}^2 \cdot \text{s})
$$

The flow of $1.7 \times 10^{-9} \text{ kg/(m}^2 \cdot \text{s})$ occurs from one element to the element directly above it, i.e. through the cross-sectional area of $15 \text{ m}^2$, corresponding to the rate of $2.6 \times 10^{-8} \text{ kg/s}$. This value is close to the flow rate given by TOUGH2 at the end of
Figure 5.25: Pore pressure profiles at different times for the single phase flow in an environment with high permeability. The pore pressure changes are now felt in the entire column and a steady state flow of water through the rock column becomes established.

1,000 years, which is $3.1 \times 10^{-8}$ kg/s. The small difference is likely to be due to the boundary conditions which assumed no flow across the side boundaries.

As the boundary conditions affect the flow in the rock column, their effect on the high permeability case was investigated. First, a solid boundary was placed at 900 m. It was found that pore pressure increased in all the elements, as flow out of the system was no longer allowed. The bottom boundary was then moved 3000 m lower. The effect of the boundary was still felt in the original elements, although the pore pressure increase was now less than in the previous case. Figure 5.26 shows the pore pressure profiles of the system at 100 years with different boundary conditions. Based on these results, it is recommended that constant pressure boundary conditions are used. This can be achieved by using elements with very large volumes ($V > 10^{50}$ m$^3$) at the boundary, as discussed in Section 4.3.2.2.
Figure 5.26: Comparison of boundary conditions for the single phase flow in an environment with high permeability. Constant pressure boundary conditions, i.e. the use of very large volume elements, is recommended for the rest of the studies.
5.3. FAR FIELD INVESTIGATIONS

5.3.2 Multiphase flow in a porous medium

5.3.2.1 Problem description

The difference between single and multiphase flows was then investigated by injecting air instead of water into the homogeneous low permeability rock column. The initial gas saturation of the host rock affects the migration of air, as rock with low initial gas saturation has a low relative permeability to air. Different initial saturations were therefore used to investigate their effect on the flow rate.

5.3.2.2 Results

Figure 5.27 shows the pore pressure and gas saturation profiles of the system at different times. Initially, the values for both pore pressure and gas saturation are zero in the entire column. It can be seen from the figure that, in 1,000 years, gas migrates less than 100 m away from the injection site in the rock of low permeability. The pore pressure increases slightly quicker than in the single phase problem (see Figure 5.24), as the effective permeability for air is lower than the effective permeability for water through the initially fully saturated rock. Air also moves primarily upwards due to buoyancy.

Figure 5.28 shows the pore pressure profile of the system at 500 years with different initial gas saturations. A higher initial gas saturation means that air flow away from the source is easier, and thus the pore pressure and gas saturation in the injection element remain lower.
Chapter 5. Behaviour of Repository Gas

Figure 5.27: Pore pressure and gas saturation profiles at different times for multiphase flow in an environment with low permeability. Gas migrates primarily upwards, which results in the pore pressure increasing faster in areas above the injection element than below it.

Figure 5.28: The effect of the initial gas saturation on multiphase flow in an environment with low permeability. The pressure profile of the system at 500 years is shown for host rocks with different initial gas saturations. A higher initial gas saturation results in the pore pressure and gas saturation in the injection element remaining lower.
5.3. FAR FIELD INVESTIGATIONS

5.3.3 Flow through barriers

5.3.3.1 Problem description

The effect of different rock features on water and gas migration was investigated next. Particular attention was paid to rock layers with low permeability which would initially act as barriers to fluid flow.

![Diagram showing high and low permeability rock layers](image)

Figure 5.29: Investigations into the effects of high and low permeability material layers. In this study, the location of the material boundary is varied.

The effect of different material layers on water and gas flow was investigated first. The bottom half of the column was assumed to have a low permeability, while the top half had a high permeability (see Figure 5.29a). Water was again injected into the original injection element at the rate of $1.0 \times 10^{-6}$ kg/s. This case is very similar to the case of single phase flow in an environment with low permeability, as the material boundary is several hundred metres above the injection site. The location of the material boundary was then brought closer to the injection element, as shown in Figure 5.29b. Multiphase flow was investigated by using air instead of water.

The effect of non-horizontal barrier formations was then studied. These included arrangements such as a capping formation above the injection element (Figure 5.30a) and a diagonal barrier followed by a plateau (Figure 5.30b). The non-horizontal barriers were created by dividing elements into smaller elements using vertical and horizontal
Figure 5.30: Investigations into the effects of barriers. The image shows the refined grid close to the injection element, originally shown in Figure 5.22, and the material properties of the new elements.

5.3.3.2 Results

The effect of a high permeability formation above the injection element was investigated first. Figure 5.31 shows that the pore pressure in the elements above the injection element stays slightly lower if a high permeability material is located 250 m above the injection element than in the case of a uniform rock column (for water flow through uniform rock column, refer back to Figure 5.24). This is because water is able to migrate through the highly permeable layer quickly. If the material boundary is only 100 m above the injection element, the pore pressure above the injection element drops further. The maximum pore pressure felt in the injection element is the same in all cases.

In the case of air injection, the results are very similar to those of multiphase flow in a rock with low permeability, as shown in Figure 5.32 (for air flow through uniform rock column, refer back to Figure 5.27). The pore pressure stays slightly lower in the areas above the injection element and below the material boundary. The pore pressure rises to values close to 50 MPa in both single phase and multiphase cases, but the flow of gas through the medium is much slower due to the lower effective permeability of the water-filled rock to gas.
5.3. FAR FIELD INVESTIGATIONS

**Figure 5.31:** The effect of material layers on water flow. Horizontal lines indicate the locations of the material boundaries for the different cases shown in Figure 5.29. Pore pressure in the areas above the injection element reduces if a high permeability rock layer is located above the low permeability layer.

**Figure 5.32:** The effect of material layers on gas flow. The flow of gas through the medium is much slower than the flow of water, due to the lower effective permeability of the water-filled rock to gas. The presence of a high permeability layer has, therefore, much less impact than in the case of single phase flow.
Figure 5.33: Gas saturation profile at 1,000 years demonstrating the accumulation of gas below a low permeability barrier formation (see the configuration in Figure 5.30a).

Figure 5.34: Gas saturation profile at 1500 years demonstrating the horizontal flow of gas below a low permeability barrier formation (see the configuration in Figure 5.30b).
5.3. FAR FIELD INVESTIGATIONS

The effect of non-horizontal barrier formations (see Figure 5.30) was then studied. Gas is seen to migrate upwards along the non-horizontal barriers and to accumulate at their highest point. Ordinarily, the gas would then stay there until the capillary entry pressure into the barrier formation is overcome. In this experiment, however, the effects of capillary pressure were ignored and the gas penetrates into the barrier formation, with its flow rate being determined by the permeability of the barrier rock and the driving pressure. This is shown in Figure 5.33. Horizontal movement of gas is detected when the pore pressure below the low permeability formation increases and the resulting pressure gradient pushes gas outwards in all the directions. The upward movement of gas is, however, restricted and so horizontal flow occurs. This is demonstrated in Figure 5.34.
5.3.4 Flow through faults

5.3.4.1 Problem description

High permeability features, such as faults, may provide a preferential gas pathway out of the repository. This section looks at the flow of hydrogen gas out of the repository through a single fault of high permeability. The repository was assumed to be intersected by a 100 m long vertical fault which provided a connection through an impermeable rock to a more permeable rock layer above it. The initial pore pressure and gas saturation were 3 MPa and 0.5 in the repository and 2 MPa and 0.0001 in the permeable rock layer 100 m above the repository. The permeability of the fault was assumed to be $1.0 \times 10^{-16}$ m$^2$ and the porosity 0.5 (i.e. if the fracture is assumed to occupy 2% of the total rock volume, this results in an effective porosity of 0.1 for the rock). The material and two-phase flow parameters for the problem are presented in Table 5.4.

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<td>$1.0 \times 10^{-16}$</td>
</tr>
<tr>
<td>Porosity</td>
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<td>0.5</td>
</tr>
<tr>
<td>$S_{LR}$</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$S_{GR}$</td>
<td>0.1</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 5.4: Material and two-phase flow parameters for the fracture flow investigations.

First, a simplified scenario was used in which 1D flow from the repository to the permeable layer occurred, as shown in Figure 5.35. The model represents the fault, with fixed pressure boundary conditions used at the top and bottom to represent the high permeability rock layer and repository. The boundary elements had very large volumes, and so an infinite supply of gas migrated through the fault into the permeable layer on top. No flow was allowed across the side boundaries. For simplicity, a linear relative permeability curve was utilised and capillary pressure effects ignored. Both of these are likely to result in over-estimation of gas flow rates through the fracture.

A 2D model was then used to investigate the same situation. The fault was now surrounded by impermeable rock, as shown in Figure 5.36. This was achieved by assigning the rock a zero permeability and porosity, so that no flow occurred through it. In practice, however, the permeability was set to zero, while the porosity had a very small value of $1.0 \times 10^{-10}$ in order to avoid numerical problems. Again, very large volume elements were used at the top and bottom to represent the repository and the permeable rock layer. No flow boundary conditions were used on the sides of the model.
5.3. FAR FIELD INVESTIGATIONS

Figure 5.35: Investigations into the effects of faults - 1D. Image shows the 1D problem set-up.

Figure 5.36: Investigations into the effects of faults - 2D. Image shows the 2D problem set-up.
5.3.4.2 Results

The 1D flow of hydrogen gas from the repository intersected by a fault (as shown in Figure 5.35) was investigated first. Hydrogen gas was found to migrate up the fault due to the pressure gradient. Figure 5.37 shows the position of the gas front at 50 years and 100 years. Hydrogen replaces water in the fracture and partially dissolves. The mass fraction of the dissolved hydrogen is also shown in Figure 5.37. The position of the displacement front at any particular times depends on the relative mobilities of water and gas, and the solubility of hydrogen.

Figure 5.38 shows the changes in hydrogen flux at the inlet of the fault and water flux at the top of the fault over time. The hydrogen flux entering the fault is large at early times due to the large pressure gradient. The flux reduces with time and stays low until approximately 100 years, which is when gas breaks through at the top. After breakthrough, the flux increases and, thereafter, stays almost constant. Water flux at the top of the fault starts after approximately 2 weeks when the pressure pulse reaches the top. The flux increases rapidly at first, and then stays constant while the hydrogen front advances up the fault. Hydrogen breaks through at approximately 100 years, which causes a drop in water flux. This is then followed by a long period of slow decline while the system dries out.

The comparison of the results from the 1D and 2D investigations is shown in Figures 5.39 and 5.40. The hydrogen front reaches the same position in both cases. However, the gas saturation of the fault in the 2D case is smaller than in the 1D case, as shown in Figure 5.39. This is because in the 1D case there is no flow through the side walls, and the pore pressure in the fault increases fairly quickly as hydrogen fills it. In the 2D case, fluids again do not migrate into the impermeable rock on the sides, but the pore pressure on the sides is kept constant at 2 MPa. The pore pressure in the fault would therefore increase more slowly, resulting in less hydrogen dissolving. Figure 5.40 shows that the flux of hydrogen flowing from the repository into the fault is slightly smaller in the 2D case, but follows the same pattern. The water flux through the top of the fault is identical in the two cases.
5.3. FAR FIELD INVESTIGATIONS

Figure 5.37: The propagation of the hydrogen front for the 1D configuration shown in Figure 5.35. The gas front advances upwards along the fault due to the pressure difference between the repository and the high permeability rock formation.

Figure 5.38: Mass fluxes of hydrogen and water for the 1D configuration shown in Figure 5.35.
CHAPTER 5. BEHAVIOUR OF REPOSITORY GAS

Figure 5.39: Comparison of 1D and 2D results: position of hydrogen front at 100 years.

Figure 5.40: Comparison of 1D and 2D results: mass fluxes of hydrogen and water.
5.3. FAR FIELD INVESTIGATIONS

5.3.4.3 Fracture flow in TOUGH2

TOUGH2 provides a way of modelling fluid flow through fractures using a concept called MINC, as discussed in Section 4.3.2.3. The use of MINC in the far field models was investigated. Figure 5.41 shows the pore pressure profiles of the low and high permeability rock columns described in Section 5.3.1, with fracture flow enabled in TOUGH2. The effective porosity was assumed to be 0.1, and flow through both fractures and matrix was allowed. The permeability of fractures was assumed to be the same as the permeability of the uniform rock.

The results show that the pore pressure profile of the rock column, with fracture flow enabled, is very similar to the profile when flow through uniform rock is modelled. In the case of high permeability rock, the results are almost identical. The slight skewing of the line in the case of the low permeability rock is due to the way matrix flow is modelled: allowing matrix flow in MINC results in one-dimensional flow between a fracture and the adjacent matrix block, rather than three-dimensional flow through the matrix. The TOUGH2 run times were found to be 5 - 7 times longer when using MINC, which resulted in actual run times of up to ten minutes for these very simple calculations. The following conclusions were, therefore, reached regarding MINC:

- Using MINC, only a small proportion of the rock, i.e. the volume occupied by pores in fractures, is available for fluid transport. This results in increased pore pressures. The volume of fractures and their porosity can be increased in order to increase the available volume. The matrix rock between fractures can also be made available for fluid flow, but this results in one-dimensional flow between the fracture and the adjacent matrix block rather than flow through the matrix.

- In the case of multiphase flow, gas encounters much less water in the fractures than it does in the homogeneous high permeability rock. Much less gas therefore dissolves.

- The use of MINC results in increased computational time. The TOUGH2 manual states that MINC increases the run times by approximately a factor of five, but in practice run times of up to seven times longer were required. Additionally, the division of elements into smaller concentric blocks, to account for the different fracture and matrix properties, results in a much larger (typically four to five times larger) number of elements. In the case of very large models, this would result in a significant increase in the data processing times, as well as the aforementioned increase in TOUGH2 run times.
Figure 5.41: Comparison of results using uniform rock properties and the fractured rock approach MINC. The flow through uniform rock was initially presented in Figures 5.24 and 5.25.
From the above it seems that the use of MINC involves considerable computational effort but produces results very similar to the cases in which only matrix flow is allowed. It is, therefore, recommended that MINC is not used in this project. Instead, the flow through porous media will be investigated and, if necessary, fractures can be introduced to the system one by one.

### 5.4 Conclusions

This chapter explained the key processes governing gas and groundwater flow in the repository near and far fields with the aid of simple TOUGH2 calculations. Table 5.5 lists all the simulations performed. It should be noted that the calculated values for pore pressures, flow rates etc. presented in this chapter do not represent actual values for the repository system, as many of the parameters chosen were unrealistic. The examples are intended to describe some of the two-phase flow processes and provide the reader with background information for more detailed calculations presented in Chapters 6, 7 and 8. It is recommended that no comparison between parameter values and/or results presented in this chapter and those used in later calculations are made.

<table>
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<td><strong>RESATURATION</strong></td>
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<td>Depth</td>
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<td>Permeability of repository</td>
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</tr>
<tr>
<td>Gravity</td>
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<tr>
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<tr>
<td>Gas presence</td>
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<tr>
<td>Model</td>
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<td><strong>FAR FIELD</strong></td>
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<td>Initial gas saturation</td>
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<td>Fault</td>
<td>1D, 2D</td>
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<td>Fracture approach</td>
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</tr>
</tbody>
</table>

Table 5.5: List of simulations carried out as part of the investigations presented in Chapter 5.

At first, the water flow into the air-filled repository was investigated. The resulting
pressure increase in the repository was found to be heavily dependent on the driving pressure and the permeability of the repository materials. The driving pressure depends on the repository depth. It was shown that in shallower repositories the resaturation rate is much slower than in deeper repositories. The sensitivity study indicated that the resaturation time decreases at the rate of 25 s/Pa - i.e. if the repository is located 100 m further up towards the surface, the resaturation process takes approximately a year longer. In shallower repositories we may be able to slow down the resaturation rate even further by engineering the repository vaults in a way which prevents or slows down water flow into them at early times. The repository design therefore becomes a major consideration. On the other hand, at greater depths resaturation occurs sooner and faster, and the repository design has less of an effect. The features of the surrounding host rock then determine the speed at which gas can migrate to the ground surface.

The two-phase flow calculations showed that a large part of the repository gas dissolves. The remaining gas can migrate into the surrounding host rock in a gaseous phase when the capillary entry barrier of the rock is exceeded. The rate of gas flow out of the repository is initially slow but increases rapidly if a continuous gas pathway between the repository and a rock layer of higher permeability is formed. This indicates the importance of assessing the effectiveness of both low and high permeability formations surrounding the repository.

It was also found that in host rocks with very low permeabilities, pore pressure near the gas source increases considerably. The pore pressure may become high enough to cause damage to the repository and the host rock, possibly resulting in the formation of a gas pathway. It should be noted, however, that the maximum pore pressure reached in this early stage of modelling is not indicative of the actual pore pressure increase within the repository, as gas was injected into a much smaller volume than would actually be the case. As TOUGH2 cannot be used to model mechanical deformation due to the pore pressure increase, bounding cases should be investigated to ensure that the pore pressure does not reach levels high enough to cause structural damage.

It seems that the van Genuchten-Mualem relative permeability model is the most commonly used function for the type of problem faced in geological disposal of radioactive waste, and it is therefore recommended as the preferred option for the more detailed 3D studies discussed in the following chapters. The same conclusion was previously reached by Nagra (2008) who also used this relationship in their gas migration studies. Bate et al. (2008), on the other hand, used linear relationships and simpler quadratic curves. The exact nature of the relative permeability and capillary pressure curves
5.4. **CONCLUSIONS**

needs to be defined by the user by selecting the appropriate parameters which define
the curve’s shape and cut-off points. Experimental data for relative permeability curves
in different types of rocks and different conditions exists in the literature, and should be
used to support the selection of the parameters. It should, however, be noted that the
relative permeability curves are highly dependent on the experimental conditions, and
sensitivity studies should be carried out to make sure the numerical models produce
valid results.

The examples also indicated that MINC, the approach for modelling fracture flow in
TOUGH2, may not be suitable for this project. The use of MINC resulted in an un-
reasonable increase in the TOUGH2 run times.

The repository materials and host rock in these studies were represented by a homoge-
neous material which combined the properties of the backfill and the waste packages.
More complicated 3D repository designs will be considered in the following chapters.
For these cases, much more data processing is required, and the use of MATLAB as
the post-processor is recommended. PetraSim provides a practical way of constructing
meshes and preparing input files, but its data handling capabilities are insufficient for
problems requiring large batch runs.
Chapter 6

Resaturation Calculations

Future generations will determine the timing of the backfilling and closure of the geological disposal facilities. When it becomes desirable to close the facility, the waste disposal areas and access tunnels will be filled with cementitious backfill material. Groundwater from the surrounding host rock will then gradually start to seep into the repository and fill all the void space within it. This chapter considers the repository resaturation process and estimates the time it takes for the vaults and tunnels to fill with water. Particular attention is paid to the effect of the repository design on the resaturation time.

The resaturation phase is studied using detailed 3D models of the disposal vaults and tunnels. The models take into account some of the engineering features of the vaults, such as the backfill material used to fill any gaps between waste packages and the low permeability liner used around the vaults to prevent water flow into them. The repository resaturation time indicates the time at which the gas generation processes in the repository start. The results of these studies will later be used as the starting point for gas migration calculations.

The chapter also considers the approach of representing the repository with one set of material parameters, instead of using the detailed models developed for the main resaturation studies. The results of these calculations are used to model the resaturation process of the entire repository. This simplification is done in order to avoid using the detailed models, for which two-phase flow simulations can take several days to complete.
6.1 Vault/tunnel scale resaturation calculations

In this section, detailed 3D models of the repository vault and tunnel are used to model the inflow of water from the surrounding host rock into the repository. The results of the simulations are used to calculate the repository resaturation time and to investigate the dependence of the resaturation time on the features of the repository and host rock. Three models were developed as part of the resaturation study: a vault, a large tunnel and a small tunnel. The vault is likely to be excavated in high-strength fractured crystalline rock at a depth of approximately 600 m. The tunnel design is more suited for lower-strength clay-based host rock, and it is assumed to be located at a depth of 300 m.

6.1.1 Vault and tunnel models

The disposal vaults and tunnels are collectively referred to as disposal units. The models of the disposal units account for some of the engineering features of the repository, such as the backfill material properties, the fill material of the crown space, the presence of a low-permeability vault liner and the arrangement of waste packages.

Figure 6.1 shows 2D cross sections of the 3D disposal units. The vault is expected to be located in high-strength fractured crystalline rock, where the excavation of large vaults is possible. The vault consists of a 7 × 7 array of waste packages (based on Edmunds and Shelton, 2007). The waste packages are taken to be 1.2 m tall and 1.5 m wide. A gap of 30 cm separates the waste packages vertically whilst a gap of 60 cm separates them horizontally. These gaps are filled with the backfill material, which, in the reference case, is assumed to have a permeability of $1 \times 10^{-16}$ m$^2$. The waste packages are assumed to have a very low permeability of $1 \times 10^{-21}$ m$^2$. The top of the repository can be left unfilled, or alternatively a fill material, such as sand, gravel or cementitious backfill, can be used. This space is taken to be 4.8 m tall. A permanent cementitious liner with a thickness of 30 cm and permeability of $1 \times 10^{-19}$ m$^2$ is used to line the vault throughout. The parameter values are further discussed in Appendix A. The mesh used in the vault simulations is shown in Figure 6.2.

The tunnel design is expected to be used in lower permeability and lower strength host rock. As such, the tunnel dimensions are smaller than those of the vault. Two versions of a disposal tunnel are modelled: a large tunnel with a height of 8.4 m and a small tunnel with a height of 5.4 m. The large and small tunnel consist of a 5 × 5 and 2 × 3 array of waste packages respectively, as shown in Figure 6.1. The waste package dimensions and spacing are the same as those used in the vault model. The tunnels do
Figure 6.1: Vault and tunnel cross-sections. The figure shows the array of waste packages (in green) surrounded by backfill material (grey), with the upper crown space (blue) and the vault sealed with a liner (black). Waste package dimensions and spacings remain constant for all types of repository.
not have a crown space as no package handling equipment needs to be attached to the ceiling (the waste packages are likely to be placed along the tunnel, starting from the back). Neither do the tunnels require a low-permeability liner, as the surrounding host rock is expected to be of very low permeability, typical of clay. The tunnel meshes are shown in Figure 6.3.

As the disposal units are several hundred metres long, the water flow into the mid-parts of them will be almost two dimensional. A thin slice, three waste packages deep, is therefore investigated. Furthermore, only half of the cross-section needs to be modelled due to symmetry. The material and two-phase flow properties to be used in the simulations are shown in Table 6.1. A van Genuchten relative permeability curve is used for all the repository materials, while a linear relative permeability function is adopted for the host rock. Capillary pressure effects are ignored in these calculations. The capillary pressure barrier, which would have to be exceeded before water enters the repository, is likely to be lower than the hydrostatic pressure at the depth of the repository. Capillary pressure is thus not considered to impact the resaturation times significantly.
Figure 6.3: Tunnel meshes. Waste packages (in dark blue) are surrounded with the backfill material (light blue). The tunnel designs do not incorporate a crown space or a low permeability liner due to the host rock having a low permeability and being of low strength. Only thin slices, three waste packages deep, of the tunnels are investigated, as the fluid flow into and out of the mid-parts of the tunnels is expected to be almost two dimensional.

The material and two-phase flow parameters for the base case resaturation simulations are presented in Table 6.1. The base case material parameters are also varied in order to investigate the effect of the different repository features on the resaturation times. Table 6.2 lists all the simulations performed as part of the vault/tunnel scale resaturation calculations.

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<th>Vault liner</th>
<th>Crown space</th>
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<td>Permeability (m²)</td>
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<td>$1.0 \times 10^{-16}$</td>
<td>$1.0 \times 10^{-21}$</td>
<td>$1.0 \times 10^{-19}$</td>
<td>$1.0 \times 10^{-16}$</td>
</tr>
<tr>
<td>Porosity (-)</td>
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<td>0.2</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>λ</td>
<td>-</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>$S_{LR}$</td>
<td>0.2</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$S_{GR}$</td>
<td>0.1</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Table 6.1: Material and two-phase flow parameters for the base case resaturation simulations.

The disposal units are surrounded by large areas of fully saturated rock at hydrostatic pressure. In the base case calculation the rock is assigned a high permeability to ensure constant availability of water. The disposal units are initially at atmospheric pressure and have an air saturation of 0.5. All the systems considered in this thesis are assumed to be isothermal.
6.1. VAULT/TUNNEL SCALE RESATURATION CALCULATIONS

<table>
<thead>
<tr>
<th>Variant</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>VAULT</td>
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<tr>
<td>Backfill permeability</td>
<td>$k = 1 \times 10^{-19}$ m$^2$ - $1 \times 10^{-15}$ m$^2$</td>
</tr>
<tr>
<td>Crown space permeability</td>
<td>$k = 1 \times 10^{-17}$ m$^2$ - $1 \times 10^{-13}$ m$^2$</td>
</tr>
<tr>
<td>Liner permeability</td>
<td>$k = 1 \times 10^{-20}$ m$^2$ - $1 \times 10^{-15}$ m$^2$</td>
</tr>
<tr>
<td>Liner thickness</td>
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</tr>
<tr>
<td>TUNNEL</td>
<td>total of 24 simulations</td>
</tr>
<tr>
<td>Backfill permeability</td>
<td>$k = 1 \times 10^{-19}$ m$^2$ - $1 \times 10^{-15}$ m$^2$</td>
</tr>
<tr>
<td>Host rock permeability</td>
<td>$k = 1 \times 10^{-20}$ m$^2$ - $1 \times 10^{-14}$ m$^2$</td>
</tr>
<tr>
<td>Layout</td>
<td>small and large tunnel</td>
</tr>
</tbody>
</table>

Table 6.2: List of simulations carried out as part of the vault/tunnel scale resaturation calculations.

Boundary conditions for the models include a no-flow boundary on three sides of the models due to symmetry and the fact that a thin slice of a very long vault is modelled. Neumann conditions are used at the top, bottom and right hand side boundaries, where the pore pressure is kept at the hydrostatic values (average pressure of 5.9 MPa for the vault and 2.9 MPa for the tunnels) and gas saturation at 0.0001. Gravity causes the pressure at the bottom to be the highest, whereas the lowest pressure is felt at the top of the models. Very large volume elements are used on these boundaries (see Section 4.3.2.2) to represent the infinite quantities of host rock surrounding the repository. These boundary conditions are based on the fact that the pore pressure and gas saturation in the host rock will not change significantly due to water or gas flow from the repository into the host rock or vice versa. The host rock around the repository therefore also provides an infinite source of water and a sink for gas.

6.1.2 Vault resaturation

Water flow from the host rock into the disposal vault was then modelled using TOUGH2. Figure 6.4 shows the water from the host rock entering the vault, initially from the bottom due to the high pressure gradient, and gradually filling all void space within it. As water penetrates the vault, air contained within the vault rises upwards in the backfilled vertical spaces between waste packages. As the space for air decreases, air compresses and dissolves into the groundwater. Figure 6.5 shows the decrease in air saturation in the innermost element above the waste packages. The graph indicates a sharp decrease in the gas saturation as the groundwater reaches the element after approximately 7 years. At this time, however, not all the air has dissolved or escaped from the vault, and the gas saturation remains slightly elevated for several decades. The increase in the gas saturation after around 10 years is due to the gas from areas
Figure 6.4: Resaturation of the disposal vault. The figure shows a sequence of gas saturation profiles taken at times 0.25 (top left corner), 1, 2, 4, 6, 8, 10 and 15 (bottom right corner) years. The gas saturation in the vault is initially 0.5 but decreases with time, as water from the surrounding rock flows in through the walls, ceiling and floor and dissolves and displaces air.
below the element rising upwards. As the waste packages have a very low permeability, air from within them is released at a slower rate than from the backfill.

![Figure 6.5: Gas saturation changes over time in the middle of the vault. Gas saturation in the vault is initially 0.5 but decreases sharply when water enters the element.](image)

The resaturation time of the vault is taken to be the time it takes for all the elements within the vault to reach an average of 0.95 water saturation. Figure 6.6 shows how the average gas saturation within the vault changes over time. The water saturation of 0.95 is considered to represent the resaturation time adequately, as water saturation does not reach values above 0.97. The resaturation time in the reference case is thus found to be approximately 6.5 years.

Following the vault reference case calculation, the effect of the repository materials on the resaturation time was investigated. This was achieved by varying the properties of the vault backfill, crown space and liner materials. The ranges of permeabilities studied are shown in Table 6.3. These investigations were performed in order to determine the relative sensitivity of the resaturation time to the material properties.

Figure 6.7 shows how the resaturation time depends on the permeability of the repository materials. It suggests that the permeability of the backfill has little effect on the resaturation behaviour unless a very low permeability material is chosen. It is, however, considered unlikely that the repository backfill would have a very low permeability due to its multi-functionality. The repository backfill is designed so that
Figure 6.6: Changes in the average gas saturation within the vault. The vault is taken to be fully saturated when the gas saturation drops below 5%.

Figure 6.7: The effect of the repository materials on the vault resaturation time. The base case permeabilities of backfill, liner and crown space are taken to be $1 \times 10^{-16}$ m$^2$, $1 \times 10^{-19}$ m$^2$ and $1 \times 10^{-16}$ m$^2$ respectively. The lines in the graph show variation in the resaturation time as the permeability of one material is changed whilst keeping the other two constant.
6.1. VAULT/TUNNEL SCALE RESATURATION CALCULATIONS

<table>
<thead>
<tr>
<th>Permeability (m²)</th>
<th>Backfill</th>
<th>Crown space</th>
<th>Vault liner</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$1.0 \times 10^{-19}$ - $1.0 \times 10^{-15}$</td>
<td>$1.0 \times 10^{-17}$ - $1.0 \times 10^{-13}$</td>
<td>$1.0 \times 10^{-20}$ - $1.0 \times 10^{-15}$</td>
</tr>
</tbody>
</table>

Table 6.3: Permeability ranges for the variants of the vault resaturation reference case.

its chemical properties prevent radionuclide migration from the vaults. To fulfill this requirement, a cementitious material is currently preferred. In the presence of groundwater, a cementitious material will increase the repository pH to a high value; this is considered as an important process in retaining radionuclides. It also leads to the backfill possessing an intrinsically high permeability.

Figure 6.7 also shows that the fill material of the crown space is found to have almost no effect on the resaturation time. The presence of a low permeability liner increases the resaturation time from less than a year to 6.5 years or higher.

6.1.3 Tunnel resaturation

The resaturation process of the two tunnels was then modelled. Figure 6.8 shows the dependence of the resaturation time on the permeability of the backfill for the two tunnel designs. The resaturation of the small tunnel is almost instantaneous due to its small dimensions and the absence of a low permeability liner. The resaturation time is only increased if the backfill has a very low permeability. The resaturation time for the large tunnel is found to be highly dependent on the permeability of the backfill. As already mentioned, the permeability of the backfill is likely to be fairly high, and so both tunnels resaturate in less than a year.

The resaturation process may take considerably longer if the host rock has a very low permeability and only limited amount of water is available. Figure 6.9 shows the effect the host rock permeability has on the resaturation time of the tunnels. As the tunnels are likely to be located in a very low permeability environment, the resaturation of the tunnels can take several decades.
Figure 6.8: The effect of the backfill permeability on the tunnel resaturation time. The lines in the graph show variation in the resaturation time for the large and small tunnel as the permeability of the backfill material is changed. The base case permeability of the backfill is $1 \times 10^{-16} \text{ m}^2$.

Figure 6.9: The effect of the host rock permeability on the tunnel resaturation time. The lines in the graph show variation in the resaturation time for the large and small tunnel as the permeability of the host rock is changed. In the base case, the permeability of the host rock is taken to be $1 \times 10^{-14} \text{ m}^2$. 
6.2 Repository scale resaturation calculations

Gas migration rates are affected by the properties of both the repository and the surrounding host rock. In order to simplify the gas migration modelling, the repository is sometimes represented by a single material which combines the properties of waste packages, backfill and other materials present in the repository. This ‘lumped material’ approach is often employed to ease computational load. The simulations of the two-phase resaturation calculations presented in the previous section required run times of up to six days. An alternative method is therefore sought to enable calculations which consider a large area of host rock around the repository.

6.2.1 Past approaches

Several authors have used volume-weighted averages of the backfill and waste packages as the repository material properties. In most of these studies, the waste packages are assumed to be impermeable and to have zero porosity, while the backfill is assumed to have values typical for a cementitious material. Bate et al. (2007) estimate an intrinsic permeability, \( k \), of \( 6.1 \times 10^{-17} \text{ m}^2 \) and a porosity, \( \phi \), of 0.12 for the lumped material, while Hoch and Swift (2010) derive values of \( k = 7.6 \times 10^{-17} \text{ m}^2 \) and \( \phi = 0.45 \). The difference in these values is likely to arise from the different vault designs, waste inventories and the waste package properties used.

A slightly different approach was adopted by Nagra (2008), who assumed that the repository material consisted of cement-filled waste drums, mortar, concrete and the shotcrete lining of the tunnels. Again, the waste packages were assumed to be impermeable and to have zero porosity. The volume-weighted average for the porosity was calculated to be 0.25. The permeability of the repository was, however, assumed to be \( 1 \times 10^{-15} \text{ m}^2 \). This was considered to be a conservative estimate based on the repository containing mainly cementitious materials, rather than being a volume-weighted average of the repository materials.

Other authors, such as Poller et al. (2009) and Senger et al. (2009), have treated the primary waste packages, concrete overpacks, crown space and backfill separately in their studies. A drawback of this technique is that it requires considerable computational effort. The next section presents an alternative way of deriving the repository material properties and investigates the effect of the repository design on the effective permeability.
6.2.2 Lumped model

Models for a typical vault and tunnel shown in Section 6.1.1 are used to calculate the effective permeability of the entire vault. The same material parameters as in the re-saturation reference case are used (see Table 6.1). The vault is initially fully saturated and a known pressure gradient is applied across it in the vertical direction. Above and below the vault are large areas of highly permeable rock with constant pressure conditions.

Water is injected into the bottom elements with a constant rate of $1.0 \times 10^{-3}$ kg/s, and the pressure difference drives flow through the vault. Zero flow boundary conditions are imposed on the sides. The simulation is allowed to run until steady state flow conditions are achieved. Once a steady state is reached, the flow rate can be used to calculate the effective permeability of the entire vault (i.e. the overall permeability of the lumped model). This provides the effective permeability in the vertical direction.

The effect of the repository features on the effective permeability is also investigated. Table 6.4 summarises all the experiments performed as part of the study.

<table>
<thead>
<tr>
<th>Variant</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LUMPED MATERIAL</strong></td>
<td>total of 212 simulations</td>
</tr>
<tr>
<td>Vault backfill permeability</td>
<td>$k = 1 \times 10^{-19} \text{ m}^2 - 1 \times 10^{-15} \text{ m}^2$</td>
</tr>
<tr>
<td>Vault crown space permeability</td>
<td>$k = 1 \times 10^{-17} \text{ m}^2 - 1 \times 10^{-13} \text{ m}^2$</td>
</tr>
<tr>
<td>Vault liner permeability</td>
<td>$k = 1 \times 10^{-20} \text{ m}^2 - 1 \times 10^{-15} \text{ m}^2$</td>
</tr>
<tr>
<td>Vault liner thickness</td>
<td>0 cm, 15 cm, 30 cm, 45 cm</td>
</tr>
<tr>
<td>Vault anisotropy</td>
<td>Flow in $x$ and $y$ directions</td>
</tr>
<tr>
<td>Tunnel backfill permeability</td>
<td>$k = 1 \times 10^{-19} \text{ m}^2 - 1 \times 10^{-15} \text{ m}^2$</td>
</tr>
</tbody>
</table>

Table 6.4: List of simulations carried out as part of the lumped model calculations.

6.2.2.1 Results of the vault lumped model

Darcy’s law can be used to estimate fluid flow rates in porous media. The relationship between the flow rate of water, $Q_{TOT}$ (expressed in units of kg/s) and permeability, $k$, can be expressed as:

$$Q_{TOT} = -k \frac{\rho A}{\mu} \frac{\partial P}{\partial z}$$  \hspace{1cm} (6.1)

where $\rho$ is density of water (kg/m$^3$), $A$ is the cross-sectional area through which flow occurs (m$^2$), $\mu$ is the dynamic viscosity of water (Pa·s), and $\partial P/\partial z$ is the pressure
gradient driving the fluid flow (Pa/m). As the total flow rate through the vault during steady state conditions can be obtained from the TOUGH2 simulation, we can calculate the effective permeability from:

\[ k = -Q_{\text{TOT}} \frac{\mu}{\rho A} \cdot \frac{\partial P}{\partial z} \]  \hspace{1cm} (6.2)

Using this method, the effective permeability for the base case is calculated to be \(2.7 \times 10^{-18} \text{ m}^2\) in the vertical \(z\)-direction. This is lower than the permeability of the vault obtained using the volume-weighted averaging method, \(6.9 \times 10^{-17} \text{ m}^2\). The discrepancy is caused by the low permeability liner around the vault: it occupies a very small volume compared to the other materials but has a significant effect on the flow through the vault.

Anisotropy was also studied by varying the direction of the pressure gradient. The effective permeability of the vault in the \(x\)-direction (horizontal direction across the vault) was found to be \(2.8 \times 10^{-18} \text{ m}^2\), and in the \(y\)-direction (horizontal direction along the vault) \(7.0 \times 10^{-17} \text{ m}^2\), as shown in Figure 6.10.

Figure 6.10: The lumped material is anisotropic. The effective permeability along the vault is much larger than that across it.

In order to demonstrate the usefulness of the lumped approach, the resaturation time
of the disposal vault using the lumped material properties was calculated. The resaturation time of the repository was now found to be 2.2 years. This is slightly less than the resaturation time obtained using the detailed model, i.e. 6.5 years, but of the same order of magnitude.

Analyses using a range of permeabilities for the backfill, crown space and liner were also performed in order to investigate which factors most affect the effective permeability of the vault. The permeability ranges are the same as those used for the resaturation calculations (see Table 6.3).

Figures 6.11 and 6.12 show the changes in the lumped permeabilities in the x and y-directions as the properties of the repository materials are changed. The permeability of the liner determines the effective permeability across the vault: the effective permeability varies by several orders of magnitude, from $3.1 \times 10^{-16} \text{m}^2$ to $3.0 \times 10^{-19} \text{m}^2$, depending on the permeability of the liner. The permeability of the crown space has a large impact upon the permeability along the vault: the effective permeability increases to $3.1 \times 10^{-15} \text{m}^2$ if the crown space has a permeability of $1.0 \times 10^{-14} \text{m}^2$.

The results of the vault simulations in the z-direction are shown in Figures 6.13 - 6.15. Figure 6.13 shows how the effective permeability of the vault changes as the properties of backfill, crown space and liner are changed. The figure indicates that the permeability of the vault liner has the biggest impact on the effective permeability: as the permeability of the liner is varied by five orders of magnitude, the effective permeability changes by approximately three orders of magnitude. The properties of the backfill also have a significant effect on the effective permeability. The backfill properties seem to have the largest impact when a medium-range liner permeability is used. At very low or high liner permeabilities, backfill properties have little effect. The fill material of the crown space is found to have little effect on the effective permeability, even if the space is left unfilled or filled with a higher permeability material such as crushed rock or gravel.

Figure 6.14 shows the comparison of the results obtained using TOUGH2 and volume-weighted averages. In almost all the cases averaging permeabilities leads to overestimation of the vault effective permeability by an order of magnitude or more. This is particularly true when the crown space possesses a high permeability. It is also noted that, as the liner permeability is increased, the results agree better with the volume-weighted averages. The vault liner would have a higher permeability if a shotcrete liner is used instead of a very low permeability permanent liner.
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Figure 6.11: The vault effective permeability in the x-direction. The graphs show how the permeability of the backfill, crown space and liner affect the effective permeability across the vault in the horizontal direction. The liner is found to have the biggest impact on the results.

Figure 6.12: The vault effective permeability in the y-direction. The graphs show how the permeability of the backfill, crown space and liner affect the effective permeability along the vault. The crown space is found to have the biggest impact on the results.
Figure 6.13: The effect of backfill, crown space and liner material properties on the vault effective permeability. The graphs show the effective permeability on the vertical axis and the permeabilities of the backfill and crown space on the x and y axes.
Figure 6.15 shows the results of the simulations in which the thickness of the liner was varied. The use of a low-permeability liner decreases the effective permeability of the vault by more than an order of magnitude. Changes in the effective permeability become smaller if the liner thickness exceeds 15 cm. The reference case value for the liner thickness is taken to be 30 cm.

The study shows that the effective permeability can vary by an order of magnitude or more depending on the direction of flow. The flow of water along the vault is much quicker than the flow through the vault in the vertical or horizontal directions. This is attributed to the large area occupied by the crown space and the lack of low-permeability liner in that direction. Near the ends of the vault the permeability along the vault would be close to the values in the other two directions, i.e. there is little variability in the permeability in the three directions. The experiments also indicate that a volume-weighted average permeability is likely to be several orders of magnitude higher than the actual effective permeability of the vault. This may be of importance to the far-field flow studies presented in Chapter 8.

### 6.2.2.2 Results of the tunnel lumped model

The calculation of the effective permeabilities for the two tunnels with heights of 8.4 m and 5.4 m yields results $k = 2.1 \times 10^{-18} \text{ m}^2$ and $k = 3.5 \times 10^{-18} \text{ m}^2$ respectively. The effective permeabilities of the vault and the two tunnels are therefore very similar, and the slight differences are mainly due to the different waste package to total volume ratios. The waste package to total volume ratios for the vault, large tunnel and small tunnel are 0.24, 0.35 and 0.30 respectively. The vault model has the smallest ratio, but the model also incorporates a low permeability liner which reduces the effective permeability.

Figures 6.16 and 6.17 show the changes in the effective permeability of the two tunnels as the backfill properties are varied. As backfill takes up a large volume of both tunnels, any changes in the backfill properties have a significant impact on the effective permeability. Once again, the volume-weighted averages produce a higher effective permeability than the simulations, but the differences are now smaller than in the vault cases due to the absence of the low permeability liner. The volume-weighted average permeabilities of the large and small tunnel in the base case are $6.5 \times 10^{-17} \text{ m}^2$ and $7.0 \times 10^{-17} \text{ m}^2$ respectively.
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Figure 6.14: Comparison of the vault effective permeability derived from TOUGH2 and the volume-weighted average permeability. The volume-weighted average permeability, shown as the dashed line, is found to be much higher than the permeability derived from TOUGH2 simulations.

Figure 6.15: The effect of liner thickness on the effective permeability of the vault. The backfill, liner and crown space permeabilities are taken to be $1 \times 10^{-16}$ m$^2$, $1 \times 10^{-19}$ m$^2$ and $1 \times 10^{-16}$ m$^2$, as in the base case.
6.2. REPOSITORY SCALE RESATURATION CALCULATIONS

Figure 6.16: The effect of the backfill properties on the large tunnel effective permeability. The backfill permeability can be seen to have a large impact on the results. The difference between the average permeability and the effective permeability derived from TOUGH2 is considerable and increases with increasing backfill permeability.

Figure 6.17: The effect of backfill properties on the small tunnel effective permeability. The backfill permeability can be seen to have a large impact on the results. There is a large discrepancy between the average permeability and the effective permeability derived from TOUGH2.
6.2.3 Resaturation of the entire repository

The resaturation process of the entire repository is then modelled using the lumped material permeabilities. A large model of the repository, including its access tunnels, excavated in fractured crystalline rock is used.

6.2.3.1 Repository model

The model is shown in Figure 6.18. It consists of 20 vaults which are 300 m long, 16 m high and 16 m wide. The access tunnels are assumed to be 5 m high and 5 m wide and filled with the backfill material. The vaults are separated by 50 m of host rock. A part of the mesh is shown in Figure 6.19.

![Plan view of the repository excavated in crystalline rock. Vaults are shown in green and access tunnels in purple.](image)

The material and two-phase flow parameters are shown in Table 6.5. The relative permeability curves used are the same as those in the vault and tunnel resaturation simulations. The vault lumped material properties are now used to represent the repository. The variations of the base case are listed in Table 6.6.

The vaults and backfilled tunnels are initially at atmospheric pressure and have a gas saturation of 0.5. The host rock is initially at hydrostatic pressure (with an average pore pressure of 5.9 MPa) and has a gas saturation of 0.0001. All the boundaries have a fixed pore pressure and gas saturation of 0.0001. They represent infinitely large areas of host rock and allow the flow of fluids into and out of the model.
6.2. **REPOSITORY SCALE RESATURATION CALCULATIONS**

Figure 6.19: Part of the repository mesh. Due to symmetry, only half of the repository is modelled. This image shows the mesh close to the middle of the repository, i.e. the axis of symmetry.

<table>
<thead>
<tr>
<th></th>
<th>Host rock</th>
<th>Back-fill</th>
<th>Repository</th>
<th>EDZ</th>
</tr>
</thead>
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<td>Permeability (m$^2$)</td>
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<td>$1.0 \times 10^{-16}$</td>
<td>$2.8 \times 10^{-18}$ $^*$</td>
<td>$1.0 \times 10^{-16}$</td>
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<td>Porosity (-)</td>
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<td>0.2</td>
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<td>$\lambda$</td>
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<td>0.5</td>
</tr>
<tr>
<td>$S_{LR}$</td>
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<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$S_{GR}$</td>
<td>0.1</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Table 6.5: Material and two-phase flow parameters for the repository resaturation simulations. $^*$) The permeability of the repository is taken to be $2.8 \times 10^{-18}$, $7.0 \times 10^{-17}$ and $2.7 \times 10^{-18}$ in the x, y and z-directions respectively.

### 6.2.3.2 Repository resaturation results

The repository is now found to resaturate in 1.2 years. The resaturation time is once again taken to be the time it takes for 95% of the vaults to fill with water. The difference between this time and the resaturation times derived for the vault earlier are likely to be caused by the slightly different dimensions of the model and the fact that the ends of the vaults resaturate quicker than the mid-parts. In the vault model, only the resaturation of a section in the middle of the vault was considered.

The changes in the repository pore pressure and gas saturation are shown in Figures 6.20 and 6.21. The images show how the pore pressure between the vaults decreases...
CHAPTER 6. RESATURATION CALCULATIONS

<table>
<thead>
<tr>
<th>Variant</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>REPOSITORY</td>
<td>total of 20 simulations</td>
</tr>
<tr>
<td>Layout</td>
<td>location of vaults</td>
</tr>
<tr>
<td>EDZ</td>
<td>0 m, 2 m</td>
</tr>
<tr>
<td>Host rock permeability</td>
<td>$k = 1 \times 10^{-20} \text{ m}^2 - 1 \times 10^{-14} \text{ m}^2$</td>
</tr>
</tbody>
</table>

Table 6.6: List of simulations carried out as part of the resaturation calculations.

Initially as water from the rock enters the vaults. The pore pressure and gas saturation in the vaults then gradually increase until they reach the initial conditions of the surrounding host rock.

The effect of the host rock permeability on the resaturation time of the repository is shown in Figure 6.22. Once again it is noticed that resaturation is very slow in host rocks of very low permeability. In these environments, the repository resaturation can take over a thousand years. In host rocks with a permeability of $1 \times 10^{-17} \text{ m}^2$ or higher, resaturation occurs in less than 3 years.

The difference between the resaturation time of a vault at the edge of the repository and a vault in the middle of the repository is also demonstrated in Figure 6.22. Vaults in the middle of the repository are expected to resaturate later than vaults near the repository edge where there is an infinite supply of water. The figure shows that if the host rock permeability is $1 \times 10^{-18} \text{ m}^2$ or below, the outer vault resaturates slightly quicker than the inner vault. The difference is, however, only a couple of years. Whilst the availability of water through the vault sidewalls in the middle of the repository may be restricted, there is an infinite supply of water below all the vaults. This explains why there is only a small difference between the resaturation times of the outer and inner vaults.

The effect of the EDZ was also examined. The EDZ corresponds to the zone around the repository, in which the material behaviour of the rock has changed as a result of the excavation process. Nagra and Andra (see for example Nagra, 2008) estimate the EDZ to play an important role in gas migration. It is expected to provide additional volume for gas storage and thus help maintain low repository pressures. Bate et al. (2007), on the other hand, conclude that the EDZ has little effect on the migration of gas out of a repository located in fractured rock. The ZEDEX Experiment in the Åspö Hard Rock Laboratory, Sweden, shows that the EDZ is likely to extend up to 1 m from the repository tunnel or vault (Emsley et al., 1997). The hydrogeological properties of the EDZ do not, however, change considerably. While the material properties of clay
Figure 6.20: Pore pressure changes in the repository. The pore pressure profile of the repository is shown at times 0.0 (top left), 0.1 (top right), 0.2, 0.5, 1.0, 2.0, 3.0 (bottom left) and 5.0 (bottom right) years. Pore pressure between the vaults initially decreases as water flows into the vaults.
Figure 6.21: Gas saturation changes in the repository. The gas saturation profile of the repository is shown at times 0.0 (top left), 0.1 (top right), 0.2, 0.5, 1.0, 2.0, 3.0 (bottom left) and 5.0 (bottom right) years. Gas saturation within the vaults reduces steadily as water flows in.
6.2. REPOSITORY SCALE RESATURATION CALCULATIONS

Figure 6.22: The effect of the host rock permeability on the repository resaturation time. Resaturation may take over 1,000 years in host rocks of very low permeability.

Figure 6.23: The effect of the EDZ on the repository resaturation time. The EDZ is found to have little impact on the results. The vault considered here is the inmost vault in the repository.
are completely different from those of hard rocks, the same conclusion of the EDZ not affecting gas migration considerably may apply; in these host rocks the EDZ is likely to reduce over time as a result of consolidation. A preferential pathway may, however, be formed due to microfracturing of the host rock.

In the present study, the EDZ was taken to be a 2 m deep layer surrounding the vaults in all directions. The permeability of the EDZ, in the direction along the disposal unit, was assumed to be ten times higher than the permeability of the intact host rock. The permeability of the EDZ in the other two directions was taken to be the same as that of the intact host rock. The resaturation time of the inner vault was compared to the resaturation time of the same vault when no EDZ is present. Figure 6.23 indicates that the vault resaturates slightly quicker in the presence of an EDZ. The difference is, however, very small: less than 1 year in host rocks with a permeability of $1 \times 10^{-18} \text{m}^2$ or over. As the properties of the EDZ were assumed to be very conservative, the EDZ is concluded not to affect the resaturation behaviour to a significant extent.

6.3 Conclusions

This chapter considered the resaturation process of an ILW disposal vault. In total, 276 simulations were carried out. The resaturation time of the vault was calculated to be approximately 6.5 years, but it was found that the repository materials have a large impact on the result. The presence of a low permeability liner significantly increases the resaturation time. The permeability of the liner has to be less than $1 \times 10^{-19} \text{m}^2$ and its thickness over 15 cm for it to cause a delay in the resaturation time. The large effect of the liner properties on the resaturation time should be taken into account in the vault design stage. The backfill properties and the fill material of the crown space were found to have little effect on the vault resaturation time.

A tunnel was found to resaturate within a year of the repository closure assuming constant availability of water. In reality, however, a low permeability host rock may not allow resaturation to occur this fast. Additionally, the calculations did not take into account the effects of the initial pressure drawdown area around the repository or the capillary pressure, both of which may also cause a delay in the resaturation times.

The chapter also presented a technique for estimating the effective permeability of waste disposal vaults and tunnels. The effective permeability of the vault was found to be $k = 2.7 \times 10^{-18} \text{m}^2$, which is considerably lower than the permeability of the vault.
obtained using the volume-weighted averaging method. The results indicate that the permeability of the vault liner has a considerable impact upon the effective permeability, as does the vault backfill. The lumped material was also found to be anisotropic with permeabilities of $k = 2.8 \times 10^{-18} \text{ m}^2$ and $k = 7.0 \times 10^{-17} \text{ m}^2$ in the x and y directions respectively.

The effective permeabilities for the large and small tunnel were found to be $k = 2.1 \times 10^{-18} \text{ m}^2$ and $k = 3.5 \times 10^{-18} \text{ m}^2$ respectively. In the tunnel calculations, the backfill properties were found to have a large impact on the results due to the large volume occupied by it.

The repository resaturation time was also calculated using the lumped material approach. The resaturation was found to occur slightly earlier, at 1.2 years, than when using the detailed model. For comparison, resaturation times using the effective permeabilities from Nagra (2008) and Bate et al. (2007) are 15 and 3 days respectively. The approach of representing the repository with the lumped material properties will therefore be utilised during the next stages of modelling.
Chapter 7

Near Field Gas Migration

When the repository has filled with water, processes such as corrosion start to generate gas. In a repository located in high permeability rock, gas may be able to migrate out of the repository into the host rock, and potentially find a pathway to the ground surface. In a low permeability host rock, gas may accumulate within the repository, and the resulting pressure increase may be sufficiently large to cause damage to the repository or the host rock. This chapter investigates what happens to the gas by modelling its behaviour within the disposal vaults and tunnels.

The chapter aims to predict whether, and in what quantities, gas escapes from the repository. First, calculations are provided to show that a free gas phase is likely to form. The behaviour of gas within a disposal vault is then illustrated using TOUGH2 simulations. Particular attention is paid to the potential pressure increase within the repository and the ways of managing the behaviour of gas through the repository design.

7.1 Formation of a free gas phase

This chapter investigates the behaviour of hydrogen gas within the repository, using the 3D models developed as part of the resaturation calculations (see Figures 6.1, 6.2 and 6.3). The resaturation phase has now been completed, and the conditions in the vault and tunnel are fully saturated, i.e. their pore pressure is close to the hydrostatic pressure at the depth of the repository and the initial gas saturation is very small at \( S_g = 0.0001 \). Each waste package now generates gas at the rate of \( 2 \times 10^{-11} \) kg/s, which corresponds to an overall gas generation rate of approximately 1000 m\(^3\)/yr from the repository located in fractured rock. Hoch and Swift (2010) estimated this to be the steady state hydrogen production rate, as discussed in Chapter 2.
Scoping calculations have been performed to indicate whether a free gas phase would form in the repository. Assuming the repository consists of 20 vaults, the total amount of hydrogen produced per vault is 50 m$^3$/yr. Using the molar volume of hydrogen of 0.089 kg/m$^3$, this is equivalent to a production rate of 4.5 kg/yr. The maximum amount of water in a fully saturated vault is the product of the vault volume (16 m $\times$ 16 m $\times$ 300 m), from which the volume of waste packages is deducted (20,000 m$^3$), and the total porosity (0.2), i.e. $V_{H_2O} = 1.1 \times 10^4$ m$^3$. Using Henry’s Law (see Section 3.1.2), the amount of hydrogen that can dissolve in the vault is:

$$m_{H_2} = H_{H_2} \times P_{H_2} \times V_{H_2O}$$

(7.1)

If we assume the gas pressure, $P_{H_2}$, to be the hydrostatic pressure at the depth of 500 m, 5 MPa, and the solubility of hydrogen in water, $H_{H_2}$, to be $1.5 \times 10^{-3}$ kg/m$^3$ (see Table 3.1), approximately 800 kg of hydrogen gas can dissolve. This is equivalent to less than 200 years of gas generation in the repository. As the gas generation is expected to continue for thousands of years, a free gas phase will eventually form. These calculations assume that no gas escapes from the system in gaseous or dissolved forms.

The overburden pressure at the depth of 500 m is approximately 13 MPa, assuming a rock density of 2600 kg/m$^3$. The maximum acceptable pressure for the gas phase, in order to avoid fracturing of the rock, would therefore be 13 MPa. Even at this pressure, a free gas phase would form after approximately 500 years. The following sections investigate what happens to the free gas as it accumulates within the repository and gradually find its way into the host rock.

### 7.2 Gas migration from the repository

In this chapter, the same models as in the vault and tunnel resaturation calculations are used to simulate the flow of fluids out of the vault and tunnel. The model parameters were first described in Section 6.1.1 (see, in particular, the description of the boundary conditions, the material and two-phase flow parameters for the base case in Table 6.1 and the grid in Figure 6.2). As before, the vault design is considered suitable for a fractured rock environment, while the tunnel design would be used in a low permeability clay environment. Table 7.1 lists all the simulations performed as part of the study.
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<table>
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<th>Variant</th>
<th>Range</th>
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<td>Backfill permeability</td>
<td>$k = 1 \times 10^{-19}$ m$^{-2}$ - $1 \times 10^{-15}$ m$^{-2}$</td>
</tr>
<tr>
<td>Crown space permeability</td>
<td>$k = 1 \times 10^{-17}$ m$^{-2}$ - $1 \times 10^{-13}$ m$^{-2}$</td>
</tr>
<tr>
<td>Liner permeability</td>
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<tr>
<td>Liner thickness</td>
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<tr>
<td>Host rock permeability</td>
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</tr>
<tr>
<td>Gas generation</td>
<td>steady-state rate, maximum rate</td>
</tr>
<tr>
<td>Sensitivity</td>
<td>$S_G, S_L$</td>
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<tr>
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<td>$k = 1 \times 10^{-20}$ m$^{-2}$ - $1 \times 10^{-14}$ m$^{-2}$</td>
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<tr>
<td>Gas generation</td>
<td>steady-state rate, maximum rate</td>
</tr>
<tr>
<td>Layout</td>
<td>small and large tunnel</td>
</tr>
</tbody>
</table>

Table 7.1: List of simulations carried out as part of the near field gas generation calculations.

The waste packages are vented and release hydrogen to the backfilled space above each package at the rate of $2 \times 10^{-11}$ kg/s. In the vault calculations, the pore pressure throughout the system is initially hydrostatic, with an average pore pressure of 5.9 MPa. In the tunnel calculations, the average pore pressure of 2.9 MPa is used. The following sections describe the gas accumulation within the vaults and tunnels and the migration of gas into the host rock.

7.2.1 Gas migration from the vault

First, gas accumulation within the vault, and its release into the host rock, is modelled using TOUGH2. Figure 7.1 shows a snapshot of the vault gas saturation at 500 years after the start of the gas generation phase. The gas saturation is the highest above waste packages, as the vented waste packages allow gases to escape. A free gas phase has formed and is moving upwards through the gaps between the waste packages and towards the ceiling of the vault.

Figure 7.2 demonstrates how gas escapes from a 1 m long section of the vault. The figure shows the different amounts escaping through the vault ceiling, walls and floor. Almost no gas escapes through the vault floor. After approximately 450 years, some gas is being pushed outwards through the vault walls, due to the increased pore pressure within the vault. The remaining gas rises upwards through the crown space and liner, and enters the host rock after approximately 600 years. After this, the flux out through the ceiling increases rapidly, as the gas pathway has been formed. At approximately 1,000 years, a steady state of flow from the vault into the host rock has been
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Figure 7.1: Vault gas saturation profile at 500 years. Gas sources can be seen in red. A free gas phase has formed and is moving upwards through the crown space.

established. The majority of the gas now escapes through the ceiling. From the graph, the flux of gas leaving the repository through the ceiling and walls during the steady state conditions is $4.5 \times 10^{-10}$ kg/s. This is equal to the total amount of gas generated within a unit length of the vault. Only a very small proportion of the gas dissolves.

Figure 7.3 shows the amount of water entering and leaving through different parts of the vault. At early times water is pushed out, ahead of the gas front, through the vault ceiling and walls. At the same time, water enters the vault through the floor. At 600 years there is a drop in the amount of water leaving the vault through the ceiling. This is due to the gas pathway being formed, which reduces the relative permeability of water, and thus makes water flow through the ceiling more difficult.

The overall gas and water outflow rates for the base case are shown in Figure 7.4. The dashed line indicating the flux of gas is now the superposition of the lines in Figure 7.2. Initially, water is pushed out from the vault due to the increased pore pressure caused by the gas generation. The water outflow rate starts to reduce as a pathway out of
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Figure 7.2: The flux of gas through different parts of the vault. Most of the gas escapes through the vault ceiling.

Figure 7.3: The flux of water through different parts of the vault. Most of the water is expelled through the vault ceiling and floor.
Figure 7.4: The total flow rate of gas and water out of the vault over time.

Figure 7.5: The changes in the average pore pressure in the vault over time. Pore pressure within the vault increases until a gas pathway into the host rock becomes established. The resulting pressure increase is insignificant in comparison with the hydrostatic pressure.
the vault becomes established. The peak gas outflow rate is reached at approximately 1,000 years. The pathway dries out slowly, which results in less and less water being pushed out.

Figure 7.5 shows the average pore pressure in the vault over time. The pore pressure starts to increase after a few hundred years and rises sharply due to gas generation. The peak pressure is reached at approximately 600 years. After this, the gas pathway into the host rock becomes established. The pressure then slowly reduces to a constant level during steady state flow of gas out of the repository. The peak pore pressure experienced in the vault is less than 5.9 MPa (this is an increase of less than 0.1 MPa from the initial pore pressure), indicating that there is little danger for structural damage due to pressure increase.

7.2.1.1 The effect of the repository design

This section investigates the effect of the repository design on the vault gas outflow rates. The same ranges of permeabilities as in the resaturation calculations (see Table 6.3) are used. The gas outflow rates for different backfill permeabilities are shown in Figure 7.6. The base case is indicated with the dashed line. It can be seen that the peak outflow rate is reached hundreds of years later if a very low permeability backfill material is used. The peak outflow rate is the same in all cases.

Figure 7.6 shows a jump in the \( k = 1 \times 10^{-19} \text{ m}^2 \) curve, while the other permeabilities result in much smoother lines. For the permeabilities \( k = 1 \times 10^{-18} - 1 \times 10^{-15} \text{ m}^2 \), gas is able to rise to the top of the vault and escape primarily through the ceiling. If the backfill has a very low permeability of \( k = 1 \times 10^{-19} \text{ m}^2 \), gas is unable to move freely and it accumulates close to the injection sources. This increases the pore pressure within the vault. The pore pressure increase results in gas being pushed away from the injection sources in all the directions, so that horizontal movement, as well as vertical, now occurs. Gas then migrates out through the sidewalls of the vault before the migration through the top starts. The jump in the \( k = 1 \times 10^{-19} \text{ m}^2 \) curve occurs when the flow through the ceiling eventually becomes established.

The gas outflow rates for different crown space materials are shown in Figure 7.7. It can be seen that the fill material of the crown space has little effect on the gas outflow rate.

Figure 7.8 shows how the liner permeability affects the gas outflow rate. The liner
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Figure 7.6: Gas flux out of the vault for different backfill permeabilities. The permeabilities of the crown space and liner are kept constant.

Figure 7.7: Gas flux out of the vault for different crown space permeabilities. The permeabilities of the backfill and liner are kept constant.
Figure 7.8: Gas flux out of the vault for different liner permeabilities. The permeabilities of the backfill and crown space are kept constant.

Figure 7.9: Gas flux out of the vault for different liner thicknesses. The permeabilities of the backfill, crown space and liner are kept constant.
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Figure 7.10: Gas flux out of the vault for different host rock permeabilities. Gas outflow starts later in very low permeability host rocks, but eventually reaches the same total outflow rate.

Figure 7.11: Vault average pore pressure for different host rock permeabilities. The pore pressure within the vault remains moderate in all the cases considered. The pressure increase in the base case was originally considered in Figure 7.5.
can be seen to have a significant effect on the outflow rates. In absence of a liner, the peak gas outflow rate is reached within 200 years of the start of the gas generation phase. A low permeability liner, however, increases the time at which peak outflow rate is reached by hundreds of years. In the case of a liner with a permeability of $1 \times 10^{-20} \text{ m}^2$, the peak outflow rate is reached after approximately 1,300 years.

The effect of the liner thickness on the gas outflow rate is demonstrated in Figure 7.9. The presence of a low permeability liner increases the time at which peak outflow rate is reached by 400 - 600 years, depending on the thickness of the liner. As before, if no liner is used, the peak outflow rate is reached after approximately 200 years.

Figure 7.10 shows the effect of the host rock permeability on the gas outflow rate. In all higher permeability cases, the timing of the gas outflow is very similar. However, in a very low permeability rock, gas outflow starts much later: if the permeability of the rock is typical of clay, i.e. $k = 1 \times 10^{-20} \text{ m}^2$, the peak outflow rate is reached over a thousand years later than in the other cases.

In a very low permeability rock, gases may accumulate within the vault instead of migrating out. The resulting pressure increase may be large enough to cause damage to the repository structures or fracturing of the host rock. Figure 7.11 demonstrates that this is unlikely to be the case with the gas generation rates considered in this study. The figure shows the gas outflow rates for different host rock permeabilities. In all the cases, the average pore pressure within the vault remains at a level which is only slightly higher than the hydrostatic pressure at the repository depth. The maximum pore pressure in all the cases considered is less than 6 MPa.

The permeabilities of the repository materials were kept constant for Figures 7.10 and 7.11, while the permeability of the host rock was varied. In all the cases, the gas front reaches the top of the vault at the same time. If the host rock permeability is higher than that of the liner, gas is able to migrate into the host rock easily. The curves for host rock permeabilities $k = 1 \times 10^{-14} - 1 \times 10^{-18} \text{ m}^2$, are therefore almost identical. For the host rock permeability $k = 1 \times 10^{-20} \text{ m}^2$, gas is initially prevented from entering the rock. This results in a slightly higher pore pressure within the vault than in the other three cases.

7.2.1.2 The effect of the gas generation rate

Hoch and Swift (2010) estimated the peak gas generation rate in the repository, soon
after its closure, to be approximately $1 \times 10^6 \text{m}^3/\text{yr}$. After this, the gas generation rate would reduce to the steady state level of $1000 \text{m}^3/\text{yr}$ - this was considered in the previous sections. The calculations presented in this section assume that the peak gas generation rate of $1 \times 10^6 \text{m}^3/\text{yr}$ is maintained for 100,000 years. This is done in order to evaluate the potential pressure increase within the vaults.

Figure 7.12: Gas flux out of the vault for the maximum gas generation rate.

Figure 7.12 shows the gas outflow rate from the vault for the peak gas generation rate. The maximum outflow rate is now reached after approximately 4 years, which is much sooner than in the lower gas generation case considered in Figure 7.5. The maximum rate is again equal to the total production rate within the vault. Due to the increased pore pressure within the vault, much more gas is now pushed out through the vault floor and walls than in the base case. The maximum outflow rate is established when the gas finds a pathway through the vault ceiling.

A pressure increase within the vault due to increased gas generation is considered in Figure 7.13. The pore pressure in the vault increases quickly, but starts to reduce after approximately 1 year. This is when gas starts to migrate through the vault walls and floor. The maximum pore pressure is now considerably higher, but still remains below 8 MPa. This indicates that the pore pressure within the vaults is unlikely to cause problems to the repository performance, even if the amount of gas produced is much larger than initially expected.
Figure 7.13: Vault average pore pressure for the maximum gas generation rate. The pore pressure within the vault remains moderate even in the case of an increased gas generation rate.

Figure 7.14: Vault average pore pressure for the maximum gas generation rate and host rock permeability of $1 \times 10^{-20}$ m$^2$. Even in this extreme case, the pore pressure increase remains sufficiently small not to give cause for concern.
An interesting scenario may be one which combines a high gas generation rate with a low permeability host rock. Figure 7.14 shows the average pore pressure within the vault if the host rock has a permeability of $k = 1 \times 10^{-20} \text{m}^2$ and the gas is generated at the maximum rate. A situation like this is unlikely to arise, as a low permeability host rock would most likely allow little ground water flow through it. This in turn would reduce the corrosion rates within the repository. The graph shows that the pore pressure remains below the lithostatic pressure at the depth of the disposal facility, 13 MPa. Pressure increase to a level which would cause damage to the repository structures, or fracturing of the host rock, is thus considered an unlikely event.

### 7.2.1.3 Sensitivity of the results to relative permeabilities of fluids

As explained in Chapter 3, the parameters used in the relative permeability curves can play an important role in the results. One of the factors that most affect the results is the irreducible gas saturation, i.e. the saturation at which gas becomes mobile. At very low irreducible gas saturations, little gas becomes trapped within the pores. Gas flow out of the vault would therefore start sooner than when using higher values. This is demonstrated in Figure 7.15. The figure shows that the results presented in this chapter can be considered as the bounding case: gas flow out of the vault is unlikely to start sooner than indicated. It is, however, possible that the flow would start much later.

Similarly, the irreducible water saturation is the minimum saturation required for the water to remain mobile. In saturations less than the irreducible water saturation, water would form an unconnected phase and become immobile. Figure 7.16 indicates that the value for irreducible water saturation used in the relative permeability curve has much less effect on the results than the irreducible gas saturation.
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Figure 7.15: Sensitivity of the results to the irreducible gas saturation. The irreducible gas saturation is found to have a large impact on the results.

Figure 7.16: Sensitivity of the results to the irreducible water saturation. The irreducible water saturation is found to impact the results much less than the irreducible gas saturation.
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7.2.2 Gas migration from the tunnel

The migration of gas out of the large and small tunnels was then investigated. Figure 7.17 shows the dependence of the outflow rate on the backfill permeability for the large tunnel. The dashed line indicates the base case results. The peak outflow rate is now reached at approximately 200 years. By using a slightly more or less permeable backfill, the time at which the peak outflow rate becomes established can be changed by approximately 100 years.

Figure 7.17 shows a kink in the curves for the backfill permeabilities $k = 1 \times 10^{-18} - 1 \times 10^{-15} \text{m}^2$ and a much smoother curve for the backfill permeability $k = 1 \times 10^{-19} \text{m}^2$. Figure 7.18 shows the average pore pressure within the large tunnel for different backfill permeabilities. It can be seen that the pore pressure for the backfill permeability $k = 1 \times 10^{-19} \text{m}^2$ increases to a level much above the other cases. The higher pore pressure within the tunnel results in gas being pushed out through the tunnel walls, as well as the ceiling. This results in the seemingly smoother curve, as the total outflow rate is the superposition of the outflow rates through the tunnel ceiling and walls. In all the other cases, gas leaves the tunnel through the tunnel ceiling only.

The results for the small tunnel are similar. Figure 7.19 indicates that the peak outflow rate is reached slightly before 200 years, and that a one order of magnitude change in the backfill permeability results in the change of approximately 100 years in the time at which peak outflow becomes established.

Figure 7.20 shows how the permeability of the host rock affects the outflow rate. The gas outflow rate seems to be very similar for low permeability host rocks, with $k < 1 \times 10^{-16} \text{m}^2$. These rocks have permeabilities lower than the permeability of the backfill. Due to the different two-phase flow properties of the host rock and backfill, gas initially accumulates within the tunnel. For the host rock permeability of $k = 1 \times 10^{-14} \text{m}^2$, flow from the tunnel into the repository is unrestrained. Whilst in a high permeability host rock, with $k = 1 \times 10^{-14} \text{m}^2$, the outflow rate becomes established at approximately 200 years, in lower permeability rocks the peak outflow rates are not reached until approximately 5,000 years later.

Figure 7.21 shows the average pore pressure within the small tunnel for different host rock permeabilities. As expected, the pore pressure increases more in lower permeability host rocks. The increase is, however, very small, less than 0.1 MPa.
Figure 7.17: Gas flux out of the large tunnel for different backfill permeabilities. The permeability of the host rock is kept constant at $1 \times 10^{-14}$ m$^2$.

Figure 7.18: Average pore pressure for different backfill permeabilities in the large tunnel. The pore pressure within the tunnel remains moderate in all the cases considered.
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Figure 7.19: Gas flux out of the small tunnel for different backfill permeabilities. The permeability of the host rock is kept constant at $1 \times 10^{-14} \text{ m}^2$.

Figure 7.20: Gas flux out of the small tunnel for different host rock permeabilities. The permeability of the tunnel backfill is kept constant at $1 \times 10^{-16} \text{ m}^2$. 
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Figure 7.21: Average pore pressure for different host rock permeabilities in the small tunnel. The pore pressure within the tunnel remains moderate in all the cases considered.

7.3 Conclusions

This chapter considered the behaviour of gas produced in the repository after its closure. Hand calculations were carried out to show that a free gas phase is likely to form within the repository. The behaviour of the gas was then simulated using TOUGH2. In total, 65 simulations were performed. It was found that some gas initially escapes through the vault walls, but that the majority of the gas leaves through the vault ceiling. A gas pathway between the repository and the host rock becomes established after approximately 600 years. After this, the flow of gas into the host rock increases until steady state flow conditions are reached at approximately 1,000 years.

The effect of the repository design on the behaviour of gas was also investigated. It was found that the presence of a low permeability liner significantly delays the start of the gas flow into the host rock. The use of a low permeability liner can result in the peak outflow rate being reached a thousand years later than when no liner is present. It was also found that the thicker the liner is, the later the gas escapes. It should be remembered, however, that the above results show the relative effect of different designs on the gas outflow rate. The chapter did not attempt to predict the exact times at which gas outflow starts.

The permeability of the host rock was found to have little effect on the gas outflow
rate, unless the repository is located in a very low permeability environment, with \( k < 1 \times 10^{-20} \text{m}^2 \). The results also indicated that the pore pressure increase within the vault is likely to be minimal, even if the repository is located in a very low permeability rock.

The potential pressure increase within the repository was evaluated by increasing the gas generation rate by three orders of magnitude. The pore pressure in the vault remained below 8 MPa in all the cases considered. This indicates that the repository performance is unlikely to be affected by a pressure increase due to gas generation.

The assessments of gas outflow from tunnels showed that the peak outflow rate is reached much sooner, at approximately 200 years. Whilst the timing could be affected by the choice of backfill by approximately 100 years, the largest impact comes from the location of the repository: a very low permeability host rock could delay the outflow of gases by thousands of years. Even in this case, however, the pore pressure within the tunnel does not increase significantly.

The impact of the parameters used in the relative permeability curves was also investigated. It was found that the value assigned for the irreducible gas saturation has a large impact on the results. The base case investigations used a very small irreducible gas saturation, implying that gas becomes mobile at very low concentrations. The results obtained here can, therefore, be considered as a bounding case; gas outflow is unlikely to start sooner than indicated.

The gas outflow rate obtained in the above calculations will be used in the next chapter. Chapter 8 will investigate what happens to the gas as it moves through the geosphere, and the properties of the host rock required to manage the gases in the long term.
Chapter 8

Far Field Gas Migration

After escaping from the repository, gas is transported through the host rock by advective and diffusive processes. This chapter studies the transport of gas in the host rock and introduces features of the host rock which are beneficial, or disadvantageous, for the management of repository gases. The area over which repository gases are released at the ground surface, the timing of the breakthrough and the maximum rate of hydrogen released in a single location are estimated. The dependence of these factors on the properties of the host rock is also investigated. The host rock is assigned different properties so that it represents either a fractured rock or a low-permeability clay environment. Additionally, other features of the host rock can affect gas migration: for example, low permeability caprock formations may act as a barrier to gas migration, while higher permeability faults may provide a preferential pathway for fluid flow. The effects of a caprock over the repository and a fault through the host rock are studied through cases in which the location and properties of these features are varied.

In the past, gas migration through the geosphere has been modelled using the detailed geology at Sellafield (see Bate et al., 2008). These kinds of specific assessments are of limited value if the actual disposal site is unknown. Other studies have looked at the behaviour of gas in different types of host rocks (see for example: Hoch and Swift, 2010; Nagra, 2008). These analyses have assumed the host rock properties to be uniform.

There have been no assessments to date which investigate the effect of generic geological features on gas migration. The investigations presented here aim to address this omission in the current safety assessments. The results aim to provide a starting point for more systematic analyses of the suitability of a host rock for radioactive waste disposal.
8.1 Far field model

The 3D far field model is shown in Figure 8.1. The repository area, within which the disposal vaults are located, is taken to be 1400 m long, 1000 m wide and 20 m high. The repository is located at a depth of 500 m. Due to symmetry, only a quarter of the repository and its surroundings need to be modelled. The dimensions of the quadrant considered are 7500 m $\times$ 2500 m $\times$ 1000 m. The results in the following sections will, however, be scaled to take into account the whole repository.

The repository is represented by a homogeneous (lumped) material, the properties of which were derived in Chapter 6. A constant gas generation rate of $1.0 \times 10^{3}$ m$^3$/yr is assumed. This amount is divided evenly between all the elements representing the repository. The repository is surrounded by the host rock with uniform material properties.

The pore pressure profile in the entire model is initially set to be hydrostatic and there is a small initial gas saturation of 0.0001. Due to symmetry, no fluid flow is allowed across the two side boundaries closest to the repository. Very large volume elements are used at the two sides furthest away from the repository, along with the top and the bottom boundaries. These elements represent infinitely large areas of host rock, with a set pore pressure and a gas saturation of 0.0001. The pore pressure in the top and bottom elements is set to be atmospheric and hydrostatic at the depth of 1000 m, i.e. 9.8 MPa, respectively. Fluid flow between the volume considered and the boundary elements is allowed.

In some calculations, the presence of a caprock layer above the repository, or a fault adjacent to the repository, is considered. These are also shown in Figure 8.1. The caprock is taken to be a 100 m thick horizontal layer of lower permeability rock, with its base placed 100 m above the top of the repository. The fault is located 100 m away from the repository. The permeability of the fault is taken to be $1.0 \times 10^{-14}$ m$^2$, and the width of the fault 1 m. In order to simplify modelling, however, the fault is represented by a larger volume with a width of 100 m and permeability of $1.0 \times 10^{-16}$ m$^2$. This approach is based on the fact that the thin theoretical fault and the wide fault used in the model have the same transmissivities. The transmissivity, $T$, of a fault is the product of the fault conductivity, $K$, and width, $e$

$$T = Ke$$  \hspace{1cm} (8.1)

The above approach is further discussed in McKeown et al. (1999). The porosity of
Figure 8.1: Far field model. The repository (in pink) is surrounded by homogeneous host rock (in light blue). Caprock is represented by the dark blue layer above the repository. A fault (in green) intersects the host rock 100 m to the right of the repository. Approximately half of the lateral extent of the model is shown here; the remaining model consists of the host rock and caprock layer.

The material parameters used in the base case far field calculations are presented in Table 8.1. The van Genuchten relative permeability and capillary pressure curves were used. It should be noted that the base case assumes the disposal site to be located in fractured rock. The permeability of the fractures may be several orders of magnitude higher than the permeability of the matrix. Fluid flow through fractures can be represented by modelling the flow through each fracture. This is, however, computationally demanding. Neuman (1990) argues that, alternatively, fractured rock can be represented by a porous medium. For simplicity, this is the approach adopted here.

A list of all the simulations to be carried out as part of the far field investigations is presented in Table 8.2. In total, 36 simulations are run. These investigate the effect
8.1. FAR FIELD MODEL

Host rock

<table>
<thead>
<tr>
<th>Property</th>
<th>Host rock</th>
<th>Repository</th>
<th>Caprock</th>
<th>Fault</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability (m²)</td>
<td>1.0 × 10⁻¹⁷</td>
<td>1.0 × 10⁻¹⁶</td>
<td>1.0 × 10⁻¹⁹</td>
<td>1.0 × 10⁻¹⁴</td>
</tr>
<tr>
<td>Porosity (-)</td>
<td>0.05</td>
<td>0.2</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>λ</td>
<td>0.6</td>
<td>0.4</td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>SLR</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>SGR</td>
<td>0.0001</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>$P_0$ (Pa)</td>
<td>1.0 × 10⁶</td>
<td>4.0 × 10³</td>
<td>1.0 × 10⁶</td>
<td>1.0 × 10⁶</td>
</tr>
</tbody>
</table>

Table 8.1: Material and two-phase flow parameters for the base case far field simulations.

of the host rock properties and features on the gas migration. In the first stage, the permeability of the host rock and repository are varied. The second stage investigates the properties of the caprock, such as its position, thickness and permeability. The final stage looks into the effect of a fault in the vicinity of the repository. The location of the fault, as well as its permeability, are varied.

For all the above cases, the effect of an increased gas generation rate is also investigated. The maximum gas generation rate was estimated by Hoch and Swift (2010) to be 1 × 10⁶ m³/yr - a value which is three orders of magnitude larger than their most realistic estimate. This value is used to evaluate the impact of a continued large gas generation rate on the results.

<table>
<thead>
<tr>
<th>Variant</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOST ROCK</td>
<td>total of 13 simulations</td>
</tr>
<tr>
<td>Repository permeability</td>
<td>$k = 1 \times 10^{-18}$ m² - $1 \times 10^{-15}$ m²</td>
</tr>
<tr>
<td>Host rock permeability</td>
<td>$k = 1 \times 10^{-20}$ m² - $1 \times 10^{-16}$ m²</td>
</tr>
<tr>
<td>Gas generation rate</td>
<td>$1 \times 10³$ m³/yr, $1 \times 10⁶$ m³/yr</td>
</tr>
<tr>
<td>CAPROCK</td>
<td>total of 13 simulations</td>
</tr>
<tr>
<td>Permeability</td>
<td>$k = 1 \times 10^{-20}$ m² - $1 \times 10^{-18}$ m²</td>
</tr>
<tr>
<td>Thickness</td>
<td>50 - 150 m</td>
</tr>
<tr>
<td>Distance from repository</td>
<td>50 - 300 m</td>
</tr>
<tr>
<td>Angle</td>
<td>0 - 10°</td>
</tr>
<tr>
<td>Gas generation rate</td>
<td>$10³$ m³/yr, $10⁶$ m³/yr</td>
</tr>
<tr>
<td>FAULT</td>
<td>total of 8 simulations</td>
</tr>
<tr>
<td>Permeability</td>
<td>$k = 1 \times 10^{-13}$ m² - $1 \times 10^{-13}$ m²</td>
</tr>
<tr>
<td>Distance from repository</td>
<td>50 - 300 m</td>
</tr>
<tr>
<td>Gas generation rate</td>
<td>$10³$ m³/yr, $10⁶$ m³/yr</td>
</tr>
</tbody>
</table>

Table 8.2: List of simulations to be carried out as part of the far field calculations.
8.2 Gas migration through uniform rock

The first stage of the modelling investigates the migration of gas through a homogeneous rock mass. Figure 8.2 presents a sequence of snapshots showing the gas saturation profile of the repository, and a part of the host rock around it, at different times. Gas is detected moving both upwards and outwards from the repository. The gas front can be seen to reach the surface between years 20,000 and 30,000. Figure 8.3 shows the average gas saturation at the ground surface over a total area of $8 \text{ km}^2$ above the repository. Gas breaks through at approximately 29,000 years.

The footprint area indicates the area over which gas can be detected at the ground surface after 100,000 years. Gas is considered to be present when the gas saturation in a single gridblock exceeds 0.001. The footprint area in the base case is found to be 2.5 km$^2$.

Figure 8.4 shows the gas saturation at the ground surface for different host rock permeabilities. The base case is indicated with the dashed line. When the permeability of the host rock is decreased, gas breaks through later. This is because in high permeability rocks gas migrates primarily upwards. In lower permeability rocks, an increased pore pressure near the gas source pushes gas outwards away from the source, so that horizontal, as well as vertical, movement occurs. Gas breakthrough time for host rock with a permeability of $k = 1 \times 10^{-19} \text{ m}^2$ is found to be 95,000 years. In the case of very low permeability host rocks, with $k \leq 1 \times 10^{-20} \text{ m}^2$, no gas is detected at the ground surface by the end of the simulation, i.e. 100,000 years.

The footprint area is found to increase slightly as the host rock permeability decreases. The maximum rate of hydrogen release at the surface is found to occur at 34,000 years. The strength of the flux is $1.7 \times 10^{-7} \text{ kg/s}$, which is the same as a yearly hydrogen release rate of 60 m$^3$.

Figure 8.5 shows the gas breakthrough time when the permeability of the repository is varied between values typical of the lumped material (see discussion in Chapter 6). The permeability of the host rock is kept constant at $1 \times 10^{-17} \text{ m}^2$. Interestingly, the breakthrough seems to occur slightly earlier, at 22,000 years, if the permeability of the repository is lower than that of the host rock, i.e. $1 \times 10^{-18} \text{ m}^2$. This supports the use of the lumped permeability concept in further investigations; the lumped permeability was found to be of the order of $1 \times 10^{-18} \text{ m}^2$. The footprint area and the maximum flux do not change significantly if the repository permeability is decreased.
Figure 8.2: Migration of gas through the uniform host rock. The figure shows a sequence of gas saturation profiles of the repository and the host rock in its vicinity. The shots are taken at 0 (top left corner), 20, 25, 30, 35 and 100 thousand years (bottom right corner). The host rock is assumed to be a homogeneous medium with a permeability of $1 \times 10^{-17}$ m$^2$. Gas can be seen to move upwards towards the ground surface and to spread laterally.
Figure 8.3: Average gas saturation at the ground surface above the repository. Gas breakthrough occurs at 29,000 years.

Figure 8.4: The effect of the host rock permeability on the gas breakthrough time. Gas does not break through in very low permeability rocks within the 100,000 year period investigated.
8.2. GAS MIGRATION THROUGH UNIFORM ROCK

Figure 8.5: The effect of the repository permeability on the gas breakthrough time.

Figure 8.6: The effect of an increased gas generation rate on the gas breakthrough time.
Figure 8.6 shows the gas breakthrough time for an increased gas generation rate. The maximum gas generation rate of $1.0 \times 10^6 \text{ m}^3/\text{yr}$ results in the hydrogen breakthrough much earlier at 240 years. The gas is found to spread to an area of $6.8 \text{ km}^2$. The hydrogen flux at the surface increases steadily over time and is $1.3 \times 10^{-4} \text{ kg/s}$ at the end of the 100,000 years.

Table 8.3 summarises the gas breakthrough times, footprint areas and maximum hydrogen fluxes at the surface for all variations of the base case. The footprint areas are found to be zero, or very small, for cases in which no gas breakthrough occurs, or in which gas breakthrough occurs close to 100,000 years.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Gas breakthrough time (years)</th>
<th>Footprint area (km$^2$)</th>
<th>Maximum flux (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Host rock permeability ($\text{ m}^2$)</td>
<td>$1.0 \times 10^{-16}$</td>
<td>26,000</td>
<td>1.6</td>
<td>$1.9 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-17}$</td>
<td>29,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-18}$</td>
<td>36,000</td>
<td>2.8</td>
<td>$1.5 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-19}$</td>
<td>95,000</td>
<td>0</td>
<td>n/a</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-20}$</td>
<td>$&gt;100,000$</td>
<td>0</td>
<td>n/a</td>
</tr>
<tr>
<td>Repository permeability ($\text{ m}^2$)</td>
<td>$1.0 \times 10^{-15}$</td>
<td>30,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-16}$</td>
<td>29,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-17}$</td>
<td>26,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-18}$</td>
<td>22,000</td>
<td>2.5</td>
<td>$1.6 \times 10^{-7}$</td>
</tr>
<tr>
<td>Gas generation rate ($\text{ m}^3/\text{yr}$)</td>
<td>$1.0 \times 10^3$</td>
<td>29,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^6$</td>
<td>240</td>
<td>6.8</td>
<td>$1.3 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Table 8.3: Summary of the results for gas migration through uniform host rock.
8.3. The effect of caprocks

In the second stage, the impact of a low permeability caprock on gas migration is investigated. The spreading of gases below and through the formation is studied, and its effect on the gas breakthrough time, footprint area and maximum hydrogen release rate at the surface are estimated.

Figure 8.7 shows how the gas saturation profile of the repository and the host rock changes between years 20,000 and 60,000. The figure demonstrates how the low permeability caprock initially traps gas beneath it. Once the capillary entry pressure of the formation has been exceeded, gas is able to penetrate into the caprock and move through it.

Figure 8.7: The trapping effect of the caprock. The images show a sequence of gas saturation profiles taken at 20 (left), 40 and 60 thousand years (right). Gas initially accumulates below the low permeability barrier, but eventually migrates through it.

Figure 8.8 shows the same behaviour as Figure 8.7, but now using 2D contour cross-sections. The images are zoomed in to show the correlation between pressure build-up below the caprock and the migration of gas.

The presence of a caprock above the repository delays the gas breakthrough at the surface, as demonstrated in Figure 8.9. A caprock with a permeability of $1 \times 10^{-18}$ m$^2$ delays the gas breakthrough time until 30,000 years, whilst a permeability of $1 \times 10^{-19}$ m$^2$ results in breakthrough at approximately 60,000 years. No breakthrough occurs before 100,000 years if a layer with a permeability less than $1 \times 10^{-20}$ m$^2$ is present.

The footprint area for the base case is found to be 2.9 km$^2$, i.e. larger than the footprint
Figure 8.8: Pore pressure and gas saturation contour plots. The contour plots represent the pore pressure and gas saturation profiles along the central plane of the repository. Note that, due to symmetry, the central plane of the repository appears on the front of the 3D model shown in Figure 8.1 (i.e. the zx-plane). The top row of images shows the pore pressure profiles due to hydrogen production after 20, 40 and 60 thousand years, while the bottom row shows the same for gas saturation.
8.3. **THE EFFECT OF CAPROCKS**

Figure 8.9: The effect of the permeability of the caprock on the gas breakthrough time. A low permeability caprock delays or prevents gas breakthrough.

Figure 8.10: The effect of the location of the caprock on the gas breakthrough time. A caprock close to the repository delays the breakthrough most effectively.
Figure 8.11: The effect of the thickness of the caprock on the gas breakthrough time. The thicker the caprock is, the later the breakthrough occurs.

Figure 8.12: Sloping caprock. The caprock (shown in dark blue) is sloping upwards away from the repository with a $10^\circ$ angle.
area for the uniform host rock. This indicates that while the caprock delays the gas breakthrough, it also spreads the gas over a slightly larger area. As the release occurs over a larger area, the maximum release rate is found to be slightly smaller than that for the uniform rock.

The properties of the capping layer were also studied. Figure 8.10 shows the results of the simulations, in which the location of the caprock was varied. The figure indicates that the closer to the repository the capping layer is, the later the gas breakthrough occurs. The breakthrough time is decreased from 60,000 years to 50,000 for the case in which the caprock is located 300 m above the repository, as opposed to 100 m in the base case. The footprint area is found to increase if the caprock is located far above the repository.

Figure 8.11 suggests that the thickness of the capping layer also has a significant effect on the breakthrough times: a 50 m thick layer results in gas breakthrough at 40,000 years, while a 150 m thick layer results in breakthrough at 65,000 years.

In order to investigate the transport of gas below a sloping barrier, a caprock was then placed at a $10^\circ$ angle to the horizontal, as shown in Figure 8.12. As mentioned earlier, the model considers a single quadrant and assumes symmetry with adjacent quadrants. As a result, the mesh in Figure 8.12 is actually modelling a slightly unrealistic scenario where two caprocks meet each other at their lowest point. This results in a 'V' shaped barrier, rather than a barrier sloping down beyond the left boundary of the mesh.

When the caprock is placed at an angle, it directs gases away from the generation site. Figure 8.13 demonstrates this. The figure shows gases accumulating below the caprock, and migrating upwards along the barrier. The gas transport below the barrier is, however, relatively slow. At approximately 55,000 years, the pore pressure below the caprock increases to a level which allows gases to move into the caprock. Gas eventually breaks through at the surface after 57,000 years. The footprint area is increased considerably for the dipping caprock - it is now $3.7\,\text{km}^2$. The maximum flux at the surface, on the contrary, does not change significantly from the base case.

Table 8.4 summarises the results of all the caprock simulations. It should be noted that the presence of a caprock delays the gas breakthrough significantly in comparison with uniform host rock. The footprint areas are, therefore, not thought to be representative of the actual areas over which gas would spread given sufficient time. In 100,000 years, gas eventually emerges at the ground surface, but only over a limited area.
Figure 8.13: The trapping effect of a dipping caprock. The images show the gas saturation profiles of the repository and host rock at 0 (top left corner), 25, 30, 35, 55 and 60 thousand years (bottom right corner). Gas migrates upwards below the low permeability barrier. The rate of removal is, however, too slow for the gases to remain trapped. At approximately 55,000 years, gas enters the caprock.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Gas breakthrough time (years)</th>
<th>Footprint area (km$^2$)</th>
<th>Maximum flux (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Caprock permeability (m$^2$)</td>
<td>$1.0 \times 10^{-18}$</td>
<td>30,000</td>
<td>2.6</td>
<td>$1.8 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-19}$</td>
<td>60,000</td>
<td>2.9</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^{-20}$</td>
<td>$&gt;100,000$</td>
<td>0</td>
<td>n/a</td>
</tr>
<tr>
<td>Location above repository (m)</td>
<td>50</td>
<td>60,000</td>
<td>2.9</td>
<td>$1.3 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>60,000</td>
<td>2.9</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>50,000</td>
<td>4.0</td>
<td>$1.2 \times 10^{-7}$</td>
</tr>
<tr>
<td>Caprock thickness (m)</td>
<td>50</td>
<td>42,000</td>
<td>2.9</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>60,000</td>
<td>2.9</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>150</td>
<td>64,000</td>
<td>2.6</td>
<td>$1.0 \times 10^{-7}$</td>
</tr>
<tr>
<td>Caprock angle (°)</td>
<td>0</td>
<td>60,000</td>
<td>2.9</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
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<td></td>
<td>10</td>
<td>57,000</td>
<td>3.7</td>
<td>$1.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>Gas generation rate (m$^3$/yr)</td>
<td>$1.0 \times 10^3$</td>
<td>60,000</td>
<td>2.9</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>$1.0 \times 10^6$</td>
<td>900</td>
<td>70.0</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 8.4: Summary of the results for gas migration through host rock with caprock overlying the repository.
8.4 The effect of faults

Finally, the effect of faults on gas migration is studied. A fault, or a backfilled access tunnel or drift, may provide a preferential pathway for gas migration; high concentrations of gas may therefore be released in a single location at the surface.

First, the fault is located 100 m away from the repository. The fault is, however, found to have little effect on the gas breakthrough time. The same result is obtained when the distance of the fault is changed to 50 m and 300 m. The gas breakthrough time, in the case of a fault at a distance of 50 m, is found to be 29,000 years, and the footprint area $2.5 \text{ km}^2$. These values are the same as those obtained for the uniform rock. This is explained by the fact that most gas migrates upwards rather than horizontally. The gas generation rate within the repository is not large enough to increase the pore pressure within the repository significantly; this would cause gas to be pushed further outwards and it would eventually reach the fault. No gas thus reaches the fault, even when the fault is located at the minimum distance of 50 m.

However, when the maximum gas generation rate of $1 \times 10^6 \text{ m}^3/\text{yr}$ is used, the gas reaches the fracture and uses it as a preferential pathway as predicted. This is shown in Figure 8.14. Gas now reaches surface before 300 years. The presence of the fault results in the maximum release rate of hydrogen of $1.2 \times 10^{-4} \text{ kg/s}$ at the ground surface. This is of similar magnitude to the maximum flux through uniform rock, but the maximum flux is now reached at approximately 500 years instead of 100,000 years as before. approximately an order of magnitude larger than the maximum flux for the uniform host rock. The maximum release rate occurs at the location where the fault ends at 500 years. The footprint area is also considerably smaller than that for the uniform host rock.

The results for the fault simulations are presented in Table 8.5. A large localised release occurs in the case of the maximum gas generation rate, potentially leading to radiological and flammability risks. It should be remembered, however, that a fault very close to the repository, and an unrealistically high gas generation rate, would be required for this behaviour to manifest itself.
Figure 8.14: The effect of a fault located at a 50 m distance from the repository. The images show the gas saturation profile of the repository and host rock at 100 (top left corner), 200, 300, 500, 1000 and 5000 (bottom right corner) years. Gas uses the fault as a preferential pathway. An unrealistically large gas generation rate and a fault close to the repository are required for this behaviour to occur.
Table 8.5: Summary of the results for gas migration through host rock, with a vertical fault intersecting the host rock.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Gas breakthrough time (years)</th>
<th>Footprint area (km²)</th>
<th>Maximum flux (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fault permeability (m²)</td>
<td>$1.0 \times 10^{-13}$</td>
<td>29,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>Distance from repository (m)</td>
<td>50</td>
<td>29,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>Gas generation rate (m³/yr)</td>
<td>$1.0 \times 10^{3}$</td>
<td>29,000</td>
<td>2.5</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

8.5 Conclusions

This chapter studied the migration of gas through the host rock. The effects of different properties and features of the host rock on gas migration were investigated, and the time at which gas emerges at the ground surface was estimated. Additionally, the area over which gas can be found at the surface after 100,000 years, and the maximum release rate of hydrogen in any single location, were calculated.

In the base case, gas was found to break through at the surface after 29,000 years. The breakthrough time depends on the permeability of the host rock; in very low permeability rocks the breakthrough time is over 100,000 years. The permeability of the repository also affects the breakthrough time: breakthrough occurs sooner for lower repository permeabilities. This supports the use of the concept of the lumped permeability, as discussed in Chapter 6, rather than a volume-weighted average permeability; in most cases, the lumped permeability was found to be much smaller than the average permeability.

The presence of a caprock delays the breakthrough time significantly: A 100 m thick caprock, with a permeability of $1 \times 10^{-19}$ m², located 100 m above the repository results in breakthrough at approximately 60,000 years. The timing is affected by the thickness, permeability and location of the caprock: the breakthrough occurs earlier if the caprock has a higher permeability, is located further away from the repository, or is thinner.

The presence of a vertical fault a minimum of 50 m away from the repository was found to have little effect on the gas breakthrough time. This was found to be the case because the gas generation rate within the repository is very small. The pore
pressure increase resulting from the gas generation would not be large enough to cause gas to be pushed outwards from the repository, and it would therefore not reach the fault. A much higher gas generation rate was required for the gas to use the fault as a preferential pathway.

In the base case, the footprint area was found to be $2.5 \text{ km}^2$. This is the area over which gas has spread at the surface after 100,000 years. The area was found to be smaller for cases in which gas breakthrough occurs later. In most simulations the footprint area remained below $3.0 \text{ km}^2$. The exceptions were the cases in which the gas generation rate was increased. A caprock located 300 m above the repository, and a caprock located at an angle, rather than a horizontal formation, were also found to spread the gas over a larger area at the surface.

For the uniform host rock base case, the maximum release rate of hydrogen at the ground surface was calculated to be $1.7 \times 10^{-7}$, i.e. $60 \text{ m}^3/\text{yr}$. The presence of a caprock was found to decrease the maximum flux; the thickness of the caprock was found to be one of the most important factors. In the case of a very low permeability host rock or caprock, no gas was found at the surface after 100,000 years. The presence of a fault had no effect on the maximum flux at the surface, unless a large gas generation rate was used.

The examples discussed in this chapter only considered the migration of gas towards the ground surface. The gas may also dissolve or be retained in the geosphere due to, for example, chemical reactions. Additionally, local groundwater flows may have a significant effect on gas migration. The calculations attempted to compare the effects of different host rock features, rather than to provide estimations of the actual gas release times and footprint areas.
Chapter 9

Conclusions

In early 2011, a radiological disaster following an earthquake and tsunami in Fukushima, Japan, caused the world’s nuclear programme to momentarily halt. As a result, the viability of nuclear power was re-evaluated throughout the world. Germany, Switzerland and Italy decided to phase out nuclear power production entirely, while the rest of the world concentrated their efforts on improving the safety and security of their nuclear installations (Schneider et al., 2011). The British new build programme was put on hold for several months but is now back on track. In order to ensure the public’s continual support to the programme, the need to demonstrate that radioactive waste disposal can be carried out safely is now more important than ever.

The current long term solution for the disposal of radioactive waste was proposed in 2006, when CoRWM recommended to the government that the waste will be placed in deep underground facilities (CoRWM, 2006). Having learnt from previous experience, a voluntarism approach between the host community and the government was to be employed. Since then, progress has been swift: a call for expressions of interest was issued out and two communities, both located in the North West close to the existing Sellafield site, applied. The call is open and other communities can join the process at any time. The site selection process will consist of in-depth desk-studies and, finally, on-site investigations. The facility is expected to be ready to receive waste in two to three decade’s time from the start of the site investigations (NDA, 2010d).

The implementation of the geological disposal facility is expected to cost approximately £3.7 billion (NDA, 2010d), making it an attractive long-term project for companies to become involved with. This EngD project was one of three research projects set up by ARUP in response to the need to increase their in-house knowledge of radioactive waste disposal. The other two projects considered public engagement and the behaviour of bentonite clay in HLW disposal facilities. ARUP were keen to demonstrate skills and
visibility within the nuclear industry. The research initiatives paid off; since 2010 ARUP have won significant contracts in both nuclear waste disposal and new build.

9.1 Overview of the project

The UK generic disposal concept introduces plans for disposing low and intermediate level waste in a repository excavated to a depth of 300 m - 1000 m. The location of the facility and the type of host rock are currently unknown. The possible disposal environments include crystalline rocks and sedimentary and evaporite rocks such as limestone, mudstone, sandstone, clays and salt. The design of the facility depends strongly on the type of host rock; the preliminary repository designs for different host rocks were published in 2011 (NDA, 2010b).

The types of waste and waste packages in the UK are expected to produce large quantities of gas in the repository conditions. Corrosion reactions are responsible for the generation of the bulk gas, hydrogen. Other gas producing reactions in the repository include, for example, radiolysis and degradation of organic waste. The amount of gas produced yearly in the repository during the steady state gas production stage is estimated to be approximately $1 \times 10^3$ m$^3$ (Hoch and Swift, 2010).

The behaviour of the repository gases has been studied in the past by modelling their migration through the repository and the host rock. These assessments were, however, very simple and treated the repository and the host rock with one set of material parameters. Alternatively they only considered one type of repository design and a specific site location. This project attempted to take a more proactive approach to gas management, by investigating the effect of the repository design and location on gas migration. Studies of the repository resaturation, along with gas migration out of the repository and through the host rock, were performed in order to estimate the relative importance of different repository and host rock features on the behaviour of gases.

The models constructed as part of the project included detailed 3D models of the disposal vault and tunnel, as well as larger models incorporating the entire repository and the surrounding host rock between the repository and the ground surface. The use of large vaults, with a height and width of approximately 16 m, is preferred in strong crystalline rocks, as they maximise the space available for disposal. A smaller tunnel design is more suited for lower strength host rocks such as clay. In these environments the tunnel diameter is estimated to be approximately 6 – 8 m. In the simulations,
the depth of the repository was varied along with the type of the host rock. Some generic properties of the host rock were incorporated into the large models, such as the presence of a caprock above the repository and a fault through the host rock. The vault and tunnel models took into account the arrangement of waste packages within the repository and the use of the backfill. The vault model additionally incorporated a low permeability liner around the vault and the presence of a crown space at the top of the vault. The properties of these features were varied in order to investigate their effect on fluid flows within and around the repository.

The gas migration modelling was carried out using a multiphase flow simulator, TOUGH2. TOUGH2 is one of only few programs available for modelling simultaneous gas and water flows, and thus commonly used in the nuclear industry. Run times of the cases presented in the thesis varied from a few minutes to several days. The models and input files were generated in PetraSim, a pre- and post-processor for TOUGH2. Data analysis was performed using MATLAB.

9.2 Summary of findings

Figure 9.1 summarises the timing of the different gas generation and migration related processes for the two potential disposal environments: a fractured crystalline rock and a low permeability rock such as clay. A vault located in a fractured rock, is expected to resaturate fairly rapidly. Gases produced within the vault are also able to migrate into the host rock easily, as the rock has a relatively high permeability. The tunnel design will be used in lower strength rocks such as clays. In these types of host environments, the permeability of the rock may be very low. A slow groundwater flow rate allows the facility to fill with water slowly, and prevents gas from entering the host rock at early times. The results from Chapters 6 - 8 for the vault and tunnel designs are summarised below.

9.2.1 Vaults in strong crystalline rocks

The resaturation of the vault was found, in Chapter 6, to be completed 6.5 years after of the closure of the repository. The resaturation time was found to be strongly dependent on the presence of a low permeability liner; in the absence of a liner the vault resaturated in less than a year. The liner needs to have a permeability of $1 \times 10^{-19} \text{ m}^2$ or less and to be over 15 cm thick for this behaviour to be noticed. The backfill material
properties and the fill material of the crown space were found to have little impact on the resaturation time.

![Diagram of gas-related processes within the repository](image)

Figure 9.1: The approximate timing of gas-related processes within the repository. Gas migration from a repository excavated in fractured rock (i.e. consisting of vaults) would start much earlier than gas migration from a repository located in a low strength low permeability rock (i.e. repository consisting of tunnels). Gas is also less likely to emerge at the ground surface if the disposal environment has a very low permeability.

Once the repository has resaturated, corrosion and other processes will start to generate gas, most of which will consist of hydrogen. While some of the gas dissolves, calculations provided in Chapter 7 showed that a free gas phase will also form. The gas will initially accumulate within the repository, but it will eventually migrate into the surrounding host rock.

Gas outflow from the vault was estimated to begin approximately 450 years after the start of the gas generation phase. A steady state flow of gas through the ceiling into the host rock becomes established at approximately 1,000 years. The timing was found to be strongly dependent on the properties of the backfill and liner. In the presence of a high permeability backfill and in the absence of a low permeability liner, gas outflow starts sooner. No gas outflow was detected before 200 years in any of the cases. In the presence of a very low permeability liner, gas outflow started much later, after approximately 700 years. Due to the outflow of gas, the pressure increase within the repository will remain too small to cause structural damage. This was found to be the case even in the presence of a very high gas generation rate.
The far field gas migration calculations in Chapter 8 indicated that gas will break through at the surface at 29,000 years. At the end of 100,000 years, gas could be detected over an area of 2.5 km$^2$. The timing of the gas breakthrough is, however, strongly dependent on the rock properties: The presence of a low permeability caprock was found to delay the gas breakthrough time significantly. A low permeability caprock, with a permeability of $1 \times 10^{-19}$ m$^2$ and a thickness of 100 m, located 50 – 100 m above the repository resulted in a breakthrough at 60,000 years and a footprint area of 2.9 km$^2$. A caprock located further away from the repository results in a breakthrough slightly earlier and the gas becomes distributed over a larger area.

A high permeability fault in the vicinity of the repository is found to have little effect on the gas migration. The fault was found to act as a preferential gas pathway only if it was located within a 50 m distance from the repository and a very large gas generation rate was used.

### 9.2.2 Tunnels in weaker sedimentary rocks

For the tunnel, the resaturation phase was calculated to last less than a year. The resaturation time was, however, found to depend strongly on the permeability of the host rock. As the tunnel design is likely to be utilised in a low permeability environment, where groundwater flow is slow, the resaturation process may take from several decades to hundreds or even thousands of years.

Gas outflow from a tunnel was estimated to start much sooner and to reach its peak at approximately 200 years. Again however, gas outflow starts later in lower permeability host rocks. If the host rock permeability is less than $1 \times 10^{-16}$ m$^2$, the peak outflow rate is reached after approximately 5,000 years. Gas migration through low permeability host rocks is also very slow: in host rocks with $k \leq 1 \times 10^{-20}$ m$^2$, no gas breaks through to the surface before 100,000 years.

### 9.3 Future work and closing remarks

This project compared the effects of different repository designs and locations on the behaviour of gases. The research hopes to provide an approach for actively managing repository gases, instead of assessing the suitability of a specific repository design.
9.3. FUTURE WORK AND CLOSING REMARKS

with regards to gas generation and migration. As the study did not aim to assess the suitability of a specific repository design, only generic features of the repository design and host rock were used. The scope of the work was chosen to comply with the time constraints and the capabilities of the chosen software. The work can be expanded on several areas:

- Temperature changes. The effect of temperature changes were not modelled as these were assumed to be moderate for L/ILW. The repository is expected to experience a peak in temperature during the curing of the backfill, immediately after closure. This could have an impact on the resaturation times.

- Coupling of the water inflow rate and gas generation rate. Gas can only be generated in the presence of adequate quantities of water. In very low permeability environments, water inflow rates may be too slow to sustain a continuous gas generation process. This may have a significant effect on the rates at which gas is transported away from the repository and through the host rock, and the timescales for gas generation processes.

- Mechanical effects. An increased pressure caused by gas generation may cause micro-fracturing of the host rock. This may be a particularly important process for low permeability low strength environments, in which gas migration would then occur through the fractures rather than the rock matrix. The flow through fractures may increase the gas migration rate through the host rock.

- Chemical processes. Chemical processes such as adsorption may affect gas migration both directly and indirectly. Direct effects are caused by chemical reactions between gases and the fluids, materials, rocks etc that they encounter in the disposal environment. Indirect effects arise from the changes these reactions cause on, for example, permeability and porosity.

- Variability of soils. In all the cases considered, only simple configurations, with at most two different rock-types, were used. Within the two rock-types, uniform properties were assumed. Under a certain pressure gradient, a gas front would advance through the uniform rock at a known speed. In reality, a gas front would not propagate at the same speed in all directions, as the rock properties may vary considerably. The variability of soils can be taken into account by using statistical methods to allocate the hydrogeological properties to each gridblock (see for example: Phoon, 2008; Nuttall, 2011).

- Properties of the repository materials. The vault liner was found to have an important effect on the resaturation and gas migration rates. Variability in the
liner and, to some extent, the backfill materials, would have a significant impact on the results, as fluid flow would occur through the weakest parts of the materials. Experience from tunnelling projects, and/or statistical methods as described above, could be used to account for this behaviour.
References


REFERENCES


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Appendix A

Note on Parameter Choices

This appendix contains a copy of an internal memorandum prepared by Steve Macklin at Ove Arup & Partners Ltd. It lists many of the parameters required for the near and far field studies presented in Chapters 6, 7 and 8. The memorandum has been attached in order to clarify the selection of parameter values.
APPENDIX A. NOTE ON PARAMETER CHOICES

ARUP

Memorandum

Page 1 of 10

To
Alex Chen

Reference number
77315-46/SRM

cc
Duncan Nicholson
David Whitaker
Matt Sykes

File reference

From
Steve Macklin x 53055 (3/13 Fitzroy Street)

Date
02 August 2010

Subject
Suggested tunnelling input parameters for Elina's Repository modelling

Alex,

As requested in our meeting of the 33rd July, I have put together some preliminary suggestions for input into Elina's numerical modelling for "far-field" gas flow. Further more specific input can follow if required.

In order to progress her analysis she has requested the following tunnelling related information:

1. what is a reasonable general arrangement/layout for ILW/LLW repositories
2. what should be extent of any excavation disturbance zone (EDZ)
3. what are reasonable assumptions for permanent lining thickness and permeability

The view from our meeting was that it may become apparent from Elina’s analysis that there are important interactions between repository geometry, development of the EDZ, permeability to gas/water and risks associated with adequate handling and backfilling that have as yet not been considered by the NDA. An "interaction matrix" approach (after Hudson) may be one way of identifying those interactions that are critical for future consideration.

Assumptions

The basic assumptions I have taken are:

- The repositories will be located in "generic" strong granite rock at 600m depth. I think it likely that any ground investigation will seek to locate the facility in good quality granite, avoiding where possible any discrete features such as faults or fracture/permeable intrusive bodies etc...
- we are considering three repository "types":
  1. large caverns ("vault") ~ 16m by 16m in cross section
  2. vertical shafts ("silo") ~ 35m diameter, 70m deep
  3. parallel tunnels ~ 6.5m diameter
- On account of deviator stresses and excavation damage an Excavation Disturbance Zone (EDZ) will form around the repository – this will affect the permeability assumed in Elina’s lumped model
- we should consider two support conditions for each of these three repository types:
  1. minimum temporary support only, such as rock bolts and shotcrete where required; represents a repository that is excavated and filled in a relatively short space of time
  2. robust permanent support comprising full temporary support plus a reinforced cast-in-situ concrete lining; represents a long-term filling approach, with allowance for retrievability
- Elina is using averaged permeability properties ("lumped model") for the stacked wastes and backfill material within each kind of repository and then will model re-equilibration of pore pressures around the repository and long term gas flow outwards. However advice on waste handling and back-filling issues for each repository type are not covered here.
Generic ground conditions

In a recent review of "rockfall scenarios" envisaged by Atkins for the design of H-LW storage packages, Atkins proposed three types of generic granitic rock mass classes based on NDA/NIKEX documentation: "strong, medium, and weak". Whilst there were a number of discrepancies in the recommended properties reported, the following parameters for the intact rock were suggested for the three generic granitic rock masses:

<table>
<thead>
<tr>
<th></th>
<th>Density Mfin⁻¹</th>
<th>Cohesion MPa</th>
<th>Phi deg</th>
<th>UCS MPa</th>
<th>Young's Modulus GPa</th>
<th>Poisson’s Ratio</th>
<th>Modulus ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong Granite</td>
<td>0.260</td>
<td>64</td>
<td>51</td>
<td>325</td>
<td>73GPa</td>
<td>0.39</td>
<td>218</td>
</tr>
<tr>
<td>Granite</td>
<td>0.255</td>
<td>45</td>
<td>44</td>
<td>170</td>
<td>47GPa</td>
<td>0.20</td>
<td>276</td>
</tr>
<tr>
<td>Weak Granite</td>
<td>0.0226</td>
<td>13</td>
<td>30</td>
<td>55</td>
<td>8GPa</td>
<td>0.10</td>
<td>145</td>
</tr>
</tbody>
</table>

Table 1 Atkins suggested intact properties for generic granite rock mass

These values are however suggesting higher than typical intact strengths and lower modulus ratios than I would expect. I have thus reviewed some recent projects I have been involved in for some further guidance.

In Hong Kong there has been a lot of underground excavation work in the medium to coarse grained Jurassic granite. The granite is frequently intruded by Tertiary basalt dykes up to 1.5m wide, 300m in length. A regional system of NE-SW trending faults also cross cut the granite forming part of the island and Kowloon Peninsula. An orthogonal system of small scale joints is prevalent and near the surface high persistence sheeting joints may be encountered. Q-index values of between 4 and 40 are typical, although it is reasonable to expect that values would approach the higher range of at depths of up to 800m, well beyond the effects of weathering and erosional stress relief. "Representative" conditions in Hong Kong are considered to lie in the range Q = 7 to 20. Intact rock strength for "firm" rock is around 150 to 250MPa. Rock mass permeability's are typically <1E-07 m/sec in good rock. Caverns spans are usually limited to 30m.

The Lake Mead (Nevada) Intake shaft cavern was recently constructed at approximately 200m depth in foliated pre- Cambrian amphibolite/gneiss. The mean strength of the rock was 150MPa. The rock mass had three well defined approximately orthogonal joint sets. Q-index values ranged from 2 to 20 for the general rock mass. Discrete fault features were estimated to have Q values ranging between 0.1 to 0.2 (GSI = 20 to 30). In situ stress ratios were unknown, but considered to be in the range 0.5 to 2. A design permeability of 1E-06 m/sec was assumed. The cavern was approximately 60m in length, 15m span and 10m in height.

The recently constructed 7-Line 34th Street Cavern in New York was excavated at a relatively shallow depth of 14m within the foliated Cambrian Schist (gneissic, schist, amphibolite and "massive" gneiss). Residual tectonic maximum stress ratios range between 2 to 12 – i.e. very high horizontal stresses. Three systematic joint sets (one parallel to schistosity) and occasional fault/shear zones are encountered. Design Q indices between 1 and 3 and GSI values 50 to 60 are typical for the general rock mass. A design intact strength of 70MPa and rock mass stiffness of 2GPa were assumed. Chlorite schist fault/shear zones are assigned the properties: rock strength = 5MPa; GSI = 20 to 40. The cavern span is 22m.

The Long Island Railroad terminus beneath Grand Central Terminal Station, New York is currently under construction. This is located within the Cambro-Ordovician Hartland Formation, a foliated mica-quartz-biotite schist. Q-index values range between 0.4 to 7, GSI 30 to 50. Stress ratios range between 1 to 3. A mean intact strength of around 30MPa was determined. Mass permeability was measured between 1E-05 to 1E-09 m/sec. Twin 20m span & height caverns, separated by a 12m rock pillar and with a rock cover of 12m will be excavated.

A series of underground vaults up to 12m span are being excavated at approximately 250 to 300m depth in Cambrian monzo-granite in the Mecsek Mountains, near Batapati Hungary. In a site visit of June 2009, I estimated the following parameters: intact strength 175MPa; GSI = 6; GSI = 60. High water inflows of up to 650L per min/100m of tunnel were being recorded at this site – for a 100m length of 5m diameter tunnel, and a hydraulic head of 250m, this would suggest
an average rock mass permeability of around 3E-07m/sec. Table 2 provides a typical classification for inflows as follows:

<table>
<thead>
<tr>
<th>INFLOW (L/min/m)</th>
<th>From</th>
<th>to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minor</td>
<td>0</td>
<td>0.1</td>
</tr>
<tr>
<td>Moderate</td>
<td>0.1</td>
<td>0.5</td>
</tr>
<tr>
<td>Moderately large</td>
<td>0.5</td>
<td>2.0</td>
</tr>
<tr>
<td>Large</td>
<td>2.0</td>
<td>4.0</td>
</tr>
<tr>
<td>Very Large</td>
<td>4.0</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 2 IMS inflow classification

My recent expert work for the Okikoto Expert Commission found numerous reports by Posiva on the investigations for the Onkalo RCF currently under construction in Finland. This facility is being excavated in Pre-Cambrian granite/gneiss, with Q values in the range 10 to 30 which roughly equates to GSI values in the range 70 to 80 (assuming Jv/SRF = 0.5). A representative intact rock strength of 100MPa is appropriate for these rocks.

On the basis that we are assuming that the facility will be located in a competent granitic rock mass at 600m depth ("high stress, tight structure" conditions) the following assessment using the Q-index (Barton et al., 1984) approach can be adopted:

1. the location of the cavern will be in rock of sufficient strength that significant spalling or slumping will not occur; the Stress Reduction Factor (SRF) will be taken as between 2 to 5;
2. the high stress and lack of weathering are assumed to result in temporary or modest inflows. Thus a joint water rating (jw) of 0.66 to 1 is proposed;
3. an average the jw/SRF ratio is thus assumed to be 0.4
4. For an assumed range of Q values between 5 and 20 ("Fair to good rock"), Q' (after Hoek et al., 1995) can be estimated as 12 to 50
5. GSI is then estimated as 9*\log(Q') + 44, which yield GSI = 66 to 79.

The following indicative range of rock mass properties (Table 3) are thus proposed:

- Intact strength: 125 to 255MPa; mass density 0.26 ton/m³;
- Mass permeability: 1E-07m/sec²;
- Q-index: 5 to 20; Q' = 12 to 50; GSI = 66 to 79
- ROCLAB "disturbance factor" D = 0.4 to 0.6
- E_pure = 14 to 40GPa; \(\sigma_{\text{max}}\) = 32 to 76MPa
- \(\varepsilon_{\text{max}}\) = 3.34 to 6.16MPa; \(\sigma_{\text{pmax}}\) = 50.6 to 58.6

A similar calculation for discrete fault/shear zones can be made. However as there is a considerable variation in potential mass properties of fault/fracture zones, and the facility will be sited to avoid/mediate these features as far as possible, I have not assessed mass properties of fault/fracture zones here.
Generic repository geometry

I understand that, on the basis of NIREX/NDP publications on generic repositories the following excavated dimensions have been assumed:

1. Vault: 16.5 by 16.5m (an arched crown, span over rise of 1/3 will be assumed here)
2. Silo: 35m diameter, 70m deep
3. Tunnel: circular, 6.5m diameter (in reality a horseshoe shape may be preferred if drill & blast excavations methods used)

A review of the literature is recommended to look at the typical general arrangements currently being employed in similar granitic conditions at depth. For example, the publication by Renne N (2008)¹ includes articles by Akas & Antilla (VUL repository, Finland) and Olson et al (Sweden) which provide indicative layouts for a combination of potential repository shapes being considered by EINUS. However there are a great many papers available that would be useful in establishing current precedent practice. Figure 1 shows a schematic layout for the VUL repository in Finland which I think may be a good analogue.

Other relevant repositories to research will include: Onkalo [currently a research facility, Finland]; Yucca Mountain (Nevada); Kameishii (Japan); Stripp Mine (Sweden); Tonellies-Mines (France); Pribram Shaft (Czech Re.); and CLAB (Sweden). The Research facilities at Pinawa (Canada); Horonobe (Japan); Aspo (Sweden); and Grimsel (Switzerland) may also be useful. The IAEA (2001) published a useful review of worldwide activity which would be worth obtaining.

APPENDIX A. NOTE ON PARAMETER CHOICES

Excavation Disturbance zone (EDZ)

The development of an EDZ will partly be due to over-stressing of the rock around the excavation. This will be a function of cross-sectional shape; longitudinal orientation with respect to maximum and minimum stress components; and the ratio of intact and mass strength to the in situ stresses. For example, studies by Derek Martin and the Canadian URL on stress induced fracture around deep excavations in granite provide some useful information on the extent of stress induced fracturing around an excavation.

Nonetheless, the feasible extent of this component of the EDZ can be estimated using a simple elastic approximation. Whilst not modelling the progressive nature of the development of a fracture zone around the excavation, the minimum extent of fracturing can be assessed. I have used the 2D Fecoscience programme EXAMINE\(^2\). Using Hoek & Brown's original chart\(^3\) (Figure 1) I have estimated a realistic range of in situ stress ratios \((\sigma_{H} : \sigma_{V})\) of 1 to 2.5 of at depths of 600m. I have added project data and also used log-log axes to provide detail at shallow depth. At 600m depth we should be looking at a vertical stress of 16MPa; \(\sigma_{H} = 16\) to 39MPa.

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\(^3\) Hoek & Brown (1980), Underground excavations in rock, IMM, Fig. 41.
On account of the generally strong/competent rock mass conditions likely to be chosen for a repository, and the shape and dimensions of the "vault" and "silo" repositories, excavation will probably only realistically be possible using drill and blast excavation methods. It is however feasible that the "tunnel" repository could be excavated using mechanical methods although for multiple tunnels side-by-side this is unlikely to be practical or cost/programme efficient. As such it will be assumed that all types of generic repository will be formed using drill and blast excavation.

A blasting induced component to the EDZ around the excavations should be expected. For instance, a review of Japanese cavern case histories by Hibino et al. [1983]4, indicated that a 40% reduction in P-wave velocity occurred in the sidewalls of one cavern after excavation. This indicated a reduction in stiffness due to the development in new fractures upon excavation.

My observations in the Botapati excavations was that a disturbance factor D = 0.5 would be appropriate on account of poor perimeter blast control and evidence of increased seepage behind shotcrete. The approach was to use pre-grouting to reduce the permeability of the rock mass rather than impose tighter blasting control.

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APPENDIX A. NOTE ON PARAMETER CHOICES

This potential increase in permeability in the EDZ due to excavation was studied by Lin & Lee (2009)\(^5\), where they found that the shape and extent of the EDZ was strongly influenced by the dominant fracture orientation; the diameter of the excavation (the bigger the opening the greater the effect) and the depth/situ stress (the higher the stress, the greater extent).

Ramulu et al (2009)\(^6\) published the results of a detailed study of blasting effects in the sidewalls of a 60m deep, 7.5m span horseshoe shaped tunnel excavated in jointed basaltic rock (strength ~ 20 to 40 MPa, RQD 25 to 90%). They found that the extent of the EDZ was up to 4m from the sidewalls. Hoek & Karszulovic (2000)\(^7\) suggest that for drill & blast excavation in open excavations, the depth of blast damage in the rock will be between 30 to 50% of the height of the excavation which fits with Ramulu’s observations.

Also of interest is a recent paper by Zhou & Jenssen which provides an approximate method of estimating the damage by drill & blast excavation upon an existing adjacent tunnel in strong competent fractured rock. The method enables an estimate of an appropriate spacing between excavations in order to avoid blast induced damage. This will also give an indirect assessment of the extent of the blast induced EDZ if we assume that the distance to a peak particle velocity (PPV) of 600mm/sec gives an approximately limited extent of new cracking in the rock – i.e. the EDZ.

\[
\begin{align*}
PPV &= f(D/Q^{0.33})^{0.5} \\
F &= \text{decoupling factor} \\
D &= \text{actual distance} \\
Q &= \text{charge weight in kg} \\
N &= \text{site attenuation coefficient, 1.5 for our generic conditions}
\end{align*}
\]

For a typical tunnel blast area of say, 20m\(^2\) cross section a “powder factor” of around 2kg/m\(^3\) would be a reasonable assumption (Figure 3). If it is assumed a 5m deep cut is taken, yielding a 100m\(^3\) volume of rock, then 200kg of explosives is required. If we then assume that the blast is fired using say 5 different time delays in the sequence, this yield 40kg per delay charge weight\(^8\). It is normal practice to use 5 – 10kg per hole, depending on the vibration limits.

This calculation is however overly simplistic because:

- The powder factor is usually higher in the centre of the blast (“the cut”) and decreases outwards
- The number of delays can be up to 40 for large cuts, and depends on the number of boreholes used and vibration limit restrictions (further limits mean more delays required)
- For benching (i.e. drilling downwards rather than horizontally to remove lower sections to the face) requires a lower PF due to the lower degree of confinement to the blast
- Smaller powder factors and high numbers of boreholes will often be used for the perimeter holes in order to minimise the blast damage (“smooth blasting or pre-splitting”)

Nonetheless a rough assessment of the extent of a blast induced fracture zone can be made (e.g. Figure 4) which suggests that at 600mm/sec, the blast damaged zone will extend only half a metre from the boundary. This would suggest that the effects of stress differentials formed around the opening will be the over-riding factor on the development of the EDZ.

Figures 5 to 10 appended, illustrating the possible zones of overstressed rock based on an elastic analysis of the three generic repository shapes, may be used to give an initial indication of the extent of the EDZ.

\(^7\) Hoek & Karszulovic (2000), Rock mass properties for surface mines. Colorado SME.

A similar calculation for a large cross section rail tunnel: area = 120m\(^2\), 5m round, 120 holes, 20 delays, 2kg/m\(^3\) PF; = 60kg per delay.
Figure 3  Standard "powder factor" curve for blasting (Dyno-Nobel "red book")
(vertical axis = face area blasted; horizontal axis = PF).

Figure 4  Standard "powder factor" curve (F = 0.05; N = 1.5; Q = 40kg/delay)
Lining thickness and permeability

On the basis of the range of Q-index values assumed for the generic granitic rock mass, I have used Barton's empirical design chart (Figure 11) to estimate the possible support used (Table 4). For the shaft, the beneficial effects of excavating vertically are accounted for by increasing the Q-index by 5.

The results in Table 4 indicate:

- For the 16m span cavern the support is insensitive to this range of Q-indices
- Bolt length is simply a function of span
- For the vault and tunnels, the bolt lengths are roughly equivalent to the EDZ estimated using elastic methods
- For the shaft, bolt length exceeds the EDZ - the final design would be governed more by potential sliding wedges larger than the EDZ - given the 30m diameter - so it is feasible that 7m bolts may be required.

In addition, I would expect that if groundwater were being encountered, weepholes would be drilled and drainage channels installed to avoid spalling of the shotcrete. This will increase the permeability depending on the diameter, length of penetration and spacing of the weepholes drilled.
<table>
<thead>
<tr>
<th>Generic repository</th>
<th>Support type</th>
<th>Q = 5</th>
<th>Q = 20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cavern/Vault (16m span)</td>
<td>Rock bolt length</td>
<td>4m</td>
<td>4m</td>
</tr>
<tr>
<td></td>
<td>Rock bolt spacing</td>
<td>2.4m</td>
<td>2.5m</td>
</tr>
<tr>
<td></td>
<td>Shotcrete</td>
<td>5 – 9cm</td>
<td>4 - 10cm</td>
</tr>
<tr>
<td>Tunnels (6.5m span)</td>
<td>Rock bolt length</td>
<td>2.5m</td>
<td>2.5m</td>
</tr>
<tr>
<td></td>
<td>Rock bolt spacing</td>
<td>2.2m</td>
<td>“Spot”</td>
</tr>
<tr>
<td></td>
<td>Shotcrete</td>
<td>4 – 10cm</td>
<td>none</td>
</tr>
<tr>
<td>Shaft (38m diameter)</td>
<td>Rock bolt length</td>
<td>7m</td>
<td>7m</td>
</tr>
<tr>
<td></td>
<td>Rock bolt spacing</td>
<td>2.6m</td>
<td>“Spot”</td>
</tr>
<tr>
<td></td>
<td>Shotcrete</td>
<td>4 – 10cm</td>
<td>none</td>
</tr>
</tbody>
</table>

Table 4 Possible support requirements according to Q-index approach (ESR = 1)

For the case where a permanent lining is to be installed I would envisage that the temporary support indicated in Table 4 would comprise additional durability requirements – such as galvanisation, full encapsulation grouting or the use of double-corrosion protection. This would alter the overall permeability characteristics of the supported zone of rock – i.e. simple, resin grouted temporary bolts would be considerably more permeable than fully grouted DCP bolts.

For a permanent lining, typically I would expect a minimum concrete thickness of 30cm, up to 45cm to allow for constructability – i.e. pouring concrete around the rebar without voids occurring, and permanent load cases for an impermeable lining. It may be that a permanent drained lining will be required in order to keep permanent water pressures on the lining to a manageable level – otherwise the secondary lining becomes excessively robust. I would normally assume concrete permeability of the order of 1E-12m/sec or higher.

In summary, the following permeability values could be assumed as first approximation:

- Rock mass permeability: 1E-07 m/sec
- EDZ/bolted zone: 1E-06 m/sec
- Shotcrete lining with weepholes & drainage channels: 1E-08 m/sec
- Permanent concrete lining: 1E-12 m/sec
ARUP

Memorandum

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Figure 5
Vault, GSI = 66 case, K = 1 (top) and K = 2.5 (bottom); D = 0.6
Figure 6  Vault, GSI = 79 case, K = 1 (top); K = 2.5 (bottom); D = 0.4
APPENDIX A. NOTE ON PARAMETER CHOICES
Figure 9  Shaft, GSI = 66, K = 1 (top); K = 2.5 (bottom); D = 0.6
Figure 10  Shaft, GSI = 79, K = 1 (top); K = 2.5 (bottom); D = 0.4
Appendix B

Publication 1

Radioactive Gas Generation and Containment in ILW Repositories

Kuitunen, E. M. and Hicks, M. A. (2008). In the proceedings of the meeting on Securing the Safe Performance of Graphite Reactor Cores held 24th-26th November 2008 at the University of Nottingham and run under the auspices of the British Carbon Group. Edited by G. B. Neighbour. RSC Publishing. Cambridge.

ABSTRACT

Radioactive wastes placed in a repository can degrade by several mechanisms giving rise to gases. Although the bulk of the gas is expected to be hydrogen, gases labelled with radionuclides such as carbon-14 and tritium are also likely to form. The migration of these radionuclides from the repository can be retarded by the use of a barrier system, which includes the host rock, as well as engineered barriers such as waste packages and backfill. In the UK, graphite is a major source of C-14 and therefore understanding its behaviour in repository conditions is vital for safety assessments.

Keywords

Carbon-14, gas generation from wastes, multi-barrier system
INTRODUCTION

Radioactive wastes placed in the repository generate gases as they evolve. Although the bulk of the gas is expected to be hydrogen, gases labelled with radionuclides are also likely to form. This paper is a first stage towards identifying factors controlling repository gas generation, and subsequent migration and attenuation of gases in the near field, with a view to influencing future repository design.

WHAT RADIONUCLIDES ARE THERE?

Tritium

Tritium is widely distributed in radioactive wastes. It has a relatively short half-life of 12.35 years and the tritium inventory in the repository will decay to insignificant levels in a few hundred years. Tritium can be incorporated into several different gaseous species, including hydrogen and methane. Depending on a range of factors, including site geology, these gases could in theory migrate to the ground surface at a relatively rapid rate if a gas pathway becomes established. Due to this reason, and the fact that there are substantial amounts of tritium present in the repository, it is necessary to consider it as one of the radionuclides capable of causing radiological exposures. However, note that for an appropriately-sited repository, it is expected that groundwater transit times will be sufficiently long so as not to cause radiological exposures to the general public from this radioactive gas (Thorne, 2005b).

Radon-222

The long-lived radionuclide radium-226 is present in some waste streams, and it produces a continuous supply of radon as it decays. Radon-222 is the only significant gas produced by radioactive decay in ILW packages, but its short half life of only 3.82 days means that it is unlikely to migrate far from the production site. As radon-222 is a noble gas, it is not expected to react with the waste package or its contents and can migrate away from its site of production by diffusive processes.

Carbon-14

Carbon-14 is created in reactor metals primarily as a result of neutron capture by nitrogen atoms through $^{14}\text{N}(n,p)^{14}\text{C}$ reaction during operation. C-14 is also present in graphite and organic wastes. C-14 atoms can be incorporated into several different chemical forms, both inorganic and organic, which will strongly affect its behaviour in
the geosphere. While the retardation mechanisms of inorganic compounds such as carbon dioxide are rather well understood, the ways in which organic compounds migrate out of the repository are less clear. Organic compounds have low solubilities and are expected to be non-reactive in the near field. The main potential hazard from carbon 14 bearing gases produced in a repository environment, in terms of radiological dose, is thus considered to arise from organic species migrating from the repository, which, dependent on site specific features, could result in a radiological hazard to man.

Inorganic compounds considered here consist mainly of C-14 labelled carbon dioxide. The geochemical behaviour of CO$_2$ is strongly affected by the alkaline environment in which CO$_2$ reacts with materials in the repository near field to form inorganic calcium carbonate through a carbonation process. The release of C-14 from this source is then mainly controlled by the solubility and dissolution kinetics of calcium carbonate. The solubility of calcium carbonate in a solution saturated with portlandite is very low and natural analogues have been used to establish that a C-14 release from the repository would not be expected to occur (Dayal and Reardon, 1992). It is however possible that the repository conditions are very different from those of naturally occurring CO$_2$ storages and the repository CO$_2$ may be able to escape. It may also be possible for CO$_2$ to react with hydrogen to produce methane, although the carbonation reaction is expected to dominate over this reaction.

The main organic radioactive gas to be generated in the repository is expected to be methane. Methane has a low solubility and is likely to be non-reactive in the repository and in the geosphere. It can therefore be transported to the ground surface more easily than carbon dioxide, and, in the worst case scenario, may result in radiological doses to the public. Note, however, that many site specific geological features could act to retard the migration of gases generated in a repository environment, possibly for very considerable timescales such that any carbon 14 present will have decayed to insignificant levels (the half life of carbon 14 is of the order of 5000 years). Such effects of site geology need to be considered when the potential dose from repository-derived C-14 is considered in assessment studies.

**GAS GENERATION PROCESSES**

Gases, to which the above-mentioned radionuclides may become incorporated, are formed in the repository as a result of several processes, including the following:
Metal corrosion

Corrosion reactions are the main source of the bulk gas, hydrogen, in the repository. Additionally, the release of C-14 and tritium from irradiated metals can result in the formation of several different C-14 and H-3 bearing gases, such as CO₂, methane and tritiated hydrogen. The rate of release of such gases is strongly dependent on the distribution of these atoms in the metal, but also on the availability of water and oxygen, and on temperature and pH, which all affect the metal corrosion rates. Additionally, the molecular form of C-14 in the metal affects the type of gas that can be formed. If carbon is present in the metal matrix as carbides, it is thought that hydrocarbons such as methane, acetylene, ethylene and ethane can be formed when the carbides become exposed on the surface and contact groundwater. If instead elemental carbon is present, the formation of organic gases is unlikely. The exact form of C-14 atoms in metals is the subject of on-going studies.

The inventories of different metals vary along with their corrosion rates, and these factors strongly affect the gas production rates. While the initial steady production of hydrogen is expected to be caused largely by the corrosion of Magnox, this inventory is expected to become consumed within approximately one hundred years of the repository closure (Hoch and Rodwell, 2003). On the other hand, steels will continue gas generation for tens, or even hundreds, of thousands of years.

Radiolysis

Dissociation of molecules by radiation can be a significant source of gas generation in an ILW repository at early times. Water within the waste package can be subjected to radiolysis from α, β and γ- radiation and produce hydrogen. If the water contains tritium, then the hydrogen produced will also be tritiated in the corresponding proportion. Radiolysis of organic compounds present in the wastes produces a variety of gases, of which hydrogen is expected to be the most important. If the organic wastes contain C-14 atoms, these may also become incorporated into the gas.

Microbial degradation of organic wastes

The degradation of cellulose and small soluble organic molecules are considered to produce gases. Cellulose is initially hydrolysed to small organic molecules which are then degraded to produce CO₂ or CH₄. Methane is only produced in anaerobic conditions and in the absence of nitrate and sulphate ions. Nitrate and sulphate thus play a major role in preventing CH₄ production from the organic wastes.
Release of ‘trapped’ radioactive gases from graphite

It is estimated that the inventory of C-14 in solid graphite accounts for about 80% of the total C-14 inventory (Norris and McKinney, 2008), but it is uncertain whether and at what rate the C-14 could be released. Some graphite may also contain tritium. The release of C-14 bearing gases and tritium can occur as graphite degrades, or by solid-state diffusion. Marsden et al. (2002) suggest that, in repository conditions, C-14 is leached at low rates from the graphite surface. Some authors (see for example Magnusson (2002)) note that both organic and inorganic forms may be formed from graphite, and that the releases are likely to be in the form of carbon dioxide and/or methane.

IMPACT OF REPOSITORY CONDITIONS ON GAS GENERATION RATES

It may be possible to affect gas generation rates by, for example, pre-treating waste or managing repository conditions during the operational phase. Gases generated in the repository during operation are, however, expected to be removed by ventilation and are not considered here.

Gas generation rates depend strongly on the waste inventories and package types used, but the potential for radioactive gas generation by a waste type is not always dependent on the amount of radionuclides in the waste. Graphite, for example, holds a large C-14 inventory, but its gas generation capability is expected to be small compared to that of metals and organic materials. In addition to waste inventories and package types, repository conditions also play an important role, as discussed below.

Availability of water

The availability of water affects the corrosion rates of metals, thus having a direct effect on gas generation rates. Water is also required for microbial reactions; if there is little water available initially, the degradation of organic wastes during repository operation is restricted and increased amounts of gases could be produced after closure, when a repository could re-saturate with groundwater. Note that, after the onset of anaerobic conditions post-closure, the production of methane is favoured over the production of carbon dioxide.
pH

The interaction of groundwater with the cementitious backfill material is expected to cause the repository pH to rise to values of 12.5-13. In highly alkaline conditions the corrosion rates of metals and the solubility of radionuclides are considerably reduced.

Temperature

Temperature affects the corrosion rates of metals; increased temperature during the backfilling stage will cause a peak in the gas production rates. Temperature may also affect the repository pH and the solubility of repository materials. The solubility of portlandite, for example, decreases with increasing temperature. The repository pH is a result of complex interactions and may therefore not rise to values as high as calculated, thus affecting the gas generation rates. Additionally, temperature can have an impact on the microbial activity.

Microbial populations

Microbial populations degrade organic material. If only low populations are present at the time of waste emplacement, more C-14 bearing organic material is left for consumption in the anaerobic rather than aerobic conditions. This means that an increased amount of methane could be generated after the repository closure.

Pockets of anaerobicity

Pockets of anaerobicity may form in the waste packages before repository closure. This would increase the methanogenic microbial reactions and thus increase the generation rate of methane during operation.

Presence of nitrate and sulphate ions

The presence of nitrate and sulphate ions increases the populations of nitrate-reducing and sulphate-reducing microbes, and slows down the growth of microbes involved in methane production. If, in particular, nitrate levels in the wastes are significantly reduced, the methane production is expected to increase (FitzGerald et al., 2004).
BARRIERS USED TO CONTROL GAS MIGRATION

Engineered and natural barriers in and around the repository act to prevent gases from reaching the biosphere, should a free gas phase form in the repository in the post-closure period. Several countries, such as the UK, France, Germany, Switzerland, Sweden, Finland, the US, Canada and Japan, have developed their preferred methods for underground disposal of radioactive wastes. Many of these involve disposal in a low permeability environment, where the host rock provides a major barrier to gas migration. However, in environments with significant groundwater flow, the role of engineered barriers in radionuclide retardation becomes far more important.

Engineered barriers

The primary role of an Engineered Barrier System (EBS) is to contain short-lived radionuclides and to limit the long-term release of long-lived radionuclides. This can be done by controlling groundwater transport in and around the repository, by limiting radionuclide solubility, and by providing sorption surfaces for the radionuclides. An EBS consists of several possible elements. These include a suitable package in which the conditioned waste is placed, a suitable encapsulant, an appropriate backfill material, and effective sealing of the repository from the surface environment.

Waste packages

The first barrier repository gases encounter is the waste package itself and the encapsulant material used. The waste package typically comprises a steel or concrete container, within which the waste is immobilised using an immobilisation matrix such as cement grout. The main function of the waste package is to contain short-lived radionuclides until they have decayed to insignificant levels. The waste container and immobilised wasteform provide a barrier for groundwater access to the wastes, thus limiting the dissolution and transport of radionuclides with the groundwater. Containers may be vented in order to prevent the build-up of internal gases and therefore some long-lived nuclides are expected to be released with gases escaping from the waste containers.

Wastes must be converted into passively safe, solid wasteforms, which means immobilising liquids, sludges and fragmented solids. A common immobilisation matrix is cement. Cementitious materials condition the chemical environment of the wasteform to high pH values, which ensures the low solubility of many radionuclides. Additionally, a high pH environment will decrease the corrosion rates of steel containers and
thus reduce the release rate of radionuclides.

**Backfilling and sealing of the repository** After all the wastes have been emplaced in the repository, backfilling, sealing and closure is possible. A role of the backfill may be to limit groundwater flow around the wastes and to create favourable physical and chemical conditions. Lu and Conca (2003) reported that backfills are often divided into two categories: chemical backfills such as cement, iron, phosphates and MgO, and hydrological/physical backfills such as clay, salt and cement.

For the assessment studies to date of a UK repository concept, the backfill material for ILW has been assumed to consist of a cementitious material, which will act as a chemical buffer and create uniform alkaline and chemically reducing conditions. Backfill will also provide a surface for radionuclide sorption due to its relatively high porosity. Additionally, it can be used as mechanical support and as a barrier to control groundwater flow around the wastes. Another commonly used backfill material is bentonite clay. This swells on contact with water and plugs all openings, thus ensuring diffusion-controlled solute transport.

The Swedish and Finnish repository concepts use crushed rock as a backfill, with the purpose of forming a hydraulic cage around the wastes. The hydraulic cage relies on the highly permeable layer of crushed rock to form a preferential pathway for groundwater flow and thus prevent advective flow driven by hydraulic gradients through the wastes. This should result in the diffusion-controlled transport of radionuclides. The long-term behaviour of the hydraulic cage is, however, not known and the crushed rock zone could provide a preferential pathway to gases, should a release occur.

The use of magnesium oxide forms an important part of the disposal concept for the WIPP repository in the US. Sacks of MgO are to be emplaced with the waste, and the wastes will be encapsulated in the repository by creep closure of the host rock (a bedded salt) which will form a low-permeability barrier around the wastes. The MgO sacks will then break open and consume moisture and CO$_2$ that may be produced in the repository. It will also buffer the pH such that actinide solubilities are limited. About 1,000 tonnes of MgO will be placed in the repository (DOE, 2004).

After backfilling the repository, repository disposal vault entrances and exits will be sealed using low-permeability materials. Seals can also be placed at other key locations to prevent the underground tunnels, drifts and shafts from acting as preferential pathways for groundwater flow and radionuclide transport. The migration of gases into the
host rock can also be controlled; for example, by shotcreting the vault walls or grouting the most transmissive features. This may affect the rate at which gas is generated in the vault (e.g. by limiting water availability) and the rate at which generated gas then migrates out of the vaults.

REPOSITORY DESIGNS

Repository designs need to deal with complex issues, such as the containment of radioactive gases, temperature increases, and isolation of waste types which may release molecules that affect the solubility or sorption of radionuclides in the waste. After encountering the engineered barriers in the repository, gas migration will depend on the properties of the host rock and the surrounding environment. Low permeability rock surrounding the repository ensures low rates of groundwater flow and thus limits radionuclide dissolution and transport with the groundwater. Also, radioactive decay, dispersion and sorption in the host rock will limit the radionuclide migration. Several disposal concepts have been proposed internationally to deal with these issues. Hicks et al. (2008) divided these into four groups as summarised in table B.1.

SUMMARY

An ILW repository may contain a significant inventory of C-14, H-3 and Rn-222. These radionuclides may form radioactive gases that can migrate from the repository to the biosphere with the bulk gas. Due to the short half-life of Rn-222, its radiological impacts are considered negligible. Tritium has also got a relatively short half-life, and so most research concentrates on the potential release of C-14 from the repository.

Corrosion of metals in the repository produces large amounts of non-radioactive hydrogen gas, but, if metals or the surrounding water contain C-14 or H-3 atoms, these can also be released in gaseous form. The form of C-14 atoms in the metal structure plays an important role: if C-14 is present as carbides it can be hydrolysed to form methane or other hydrocarbons; if C-14 is present in its elemental form, it is unlikely to form a gas. Another possible source of radioactive gas is graphite, as it holds a substantial inventory of C-14 which may form methane in repository conditions. Understanding the release behaviour of C-14 from graphite is currently a key concern for repository safety.

Radiological waste repositories can be located in various geological settings. The properties of the surrounding rock determine the importance of engineered barriers to long term safety. If the repository is located in a low permeability host rock where there is
<table>
<thead>
<tr>
<th>Disposal in:</th>
<th>Weak rock with little or no groundwater flow</th>
<th>Strong rock with little or no groundwater flow</th>
<th>Strong rock with significant groundwater flow</th>
<th>Plastic evaporite rock with no groundwater flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Countries</td>
<td>Belgium, France, Japan, Switzerland</td>
<td>Canada, Japan</td>
<td>Sweden, Finland</td>
<td>U.S.</td>
</tr>
<tr>
<td>Host rock</td>
<td>Indurated/plastic low permeability sedimentary rock</td>
<td>Crystalline rock</td>
<td>Crystalline rock, carbonate</td>
<td>Evaporites: salt dome, bedded salt</td>
</tr>
<tr>
<td>Primary barrier</td>
<td>Host rock most important barrier. Self-healing of cracks and fissures an important property of the rock.</td>
<td>Low-permeability environment most important barrier. Importance of EBS increased if there is groundwater flow.</td>
<td>Role of EBS far more important than in other concepts. Cementitious materials limit groundwater flow and provide long-lasting alkaline environment.</td>
<td>Low permeability salt rock encloses waste as result of salt creep.</td>
</tr>
<tr>
<td>Secondary barriers</td>
<td>Alkaline and reducing environment due to cementitious materials will limit radionuclide solubility and increase sorption.</td>
<td>Alkaline and reducing environment due to cementitious materials will limit radionuclide solubility and increase sorption.</td>
<td>Host rock with low hydraulic conductivity.</td>
<td>Engineered low permeability seals will prevent shafts from becoming preferential pathways.</td>
</tr>
<tr>
<td>Waste packages</td>
<td>Concrete (sometimes bitumen) used as immobilisation matrix. Emplacement packages proposed in several concepts.</td>
<td>Several immobilisation matrices proposed. Cement often used to provide alkaline conditions.</td>
<td>Cement conditioned wastes placed in metal containers or concrete packages.</td>
<td>Steel containers used for handling rather than to perform a specific role in radionuclide retention.</td>
</tr>
<tr>
<td>Backfill</td>
<td>Grout backfill sometimes used. Sealing of disposal tunnels, caverns, etc. important in preventing these from becoming preferential pathways.</td>
<td>Rock bolts and grout (sometimes bentonite) backfill often used for mechanical stability.</td>
<td>Crushed rock used to divert flow away from waste packages.</td>
<td>MgO used as buffer to limit actinide solubilities.</td>
</tr>
</tbody>
</table>

Table B.1: Common features of repositories in different geological settings. (Based on Hicks et al. (2008)
little or no groundwater flow, the host rock can be regarded as the most important factor in radionuclide retardation. However, when groundwater flow rates are increased, engineered barriers play a much more important role.

ACKNOWLEDGEMENTS

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References


Issue 4.


Appendix C

Publication 2

Gas Migration from Nuclear Waste Repositories: Calculation of Vault Effective Permeability


**ABSTRACT**

It is envisaged that the low and intermediate level waste resulting from Britain’s nuclear power generation activities are to be placed in disposal facilities deep underground. After emplacement of waste in the disposal vaults, the facilities will be backfilled and closed. Processes such as corrosion will then result in large quantities of gas being produced within the repository vaults.

Many studies have been carried out to investigate the behaviour of the gases in the repository environment. These studies often model the vault containing the waste packages with one set of material parameters which combines the properties of the waste packages and backfill using a volume-weighted average approach. This article introduces a new way of deriving the effective permeability of the vault and examines the effect of the vault design, such as the fill material of the crown space and the permeability of the vault liner, on the calculated permeability. The work is carried out with the TOUGH2 software package.
INTRODUCTION

It has been decided that the UK low and intermediate level radioactive waste will be disposed of in deep underground facilities (CoRWM, 2006). Before the disposal can take place, the disposal sites need to be identified and safety/performance assessments carried out. Radioactive waste placed in a repository can degrade by several mechanisms, giving rise to gas generation. Although the bulk of the gas is expected to be hydrogen, the formation of radioactive gases, containing tritium, carbon-14 and radon-222 atoms, is also expected.

The types of waste and waste packages in the UK are expected to produce large quantities of gas. Corrosion reactions are responsible for the generation of the bulk gas, hydrogen. Metals present in the waste stream include, for example, magnox, irradiated uranium, stainless steels, aluminium and zircaloy from nuclear fuel cladding. The rate of the corrosion reactions depends on the availability of water and oxygen. Other gas producing reactions in the repository include, for example, radiolysis and degradation of organic waste. The amount of gas produced yearly in the repository during the steady state gas production stage is estimated to be approximately $1 \times 10^3 \text{m}^3$ (Hoch and Swift, 2010).

The behaviour of the repository gases has been studied by modelling their migration through the repository and the host rock. Modelling performed using a revised waste inventory in 2005 led to the gas pathway producing a risk in excess of the government defined target (Nirex, 2005). After this, it was clear that more research into gas generation and migration was needed. Since then, several studies have been carried out to look at the gas migration in the host rock, around the disposal vaults and in different geologies.

In many gas migration modelling studies which consider the repository and the surrounding host rock, the repository is represented using a lumped model approach. The material parameters used in the lumped model combine the properties of the waste packages and backfill. Many researchers (see for example Bate et al., 2008; Nagra, 2008) use volume-weighted averages to obtain the effective permeability of the repository materials. This study investigates the effect of the repository design on the effective permeability. A 'lumped' model for a typical vault in fractured crystalline rock is developed. The lumped model takes into account different design aspects of the repository, such as the fill material of the crown space and the hydrogeological properties of the low permeability liner used around the vaults. By taking a detailed
design of the repository vault and applying a constant pressure gradient through it, the
effective permeability of the entire vault can be estimated. This article introduces the
method used to calculate the effective permeability. Different design aspects are taken
into account by varying the properties of the backfill, crown space and vault liner.

THE GEOLOGICAL DISPOSAL FACILITY

The repository for radioactive waste will be designed so that both natural and engi-
neered features will be used to prevent radionuclides from escaping. Several countries,
such as France, Germany, Switzerland, Sweden, Finland, the U.S., Canada and Japan,
have developed their preferred methods for underground disposal of radioactive waste.
Many of these, such as the French and Swiss concepts, involve disposal in a low-
permeable environment with only little groundwater flow through it. These concepts
rely on the natural barrier, the host rock, to prevent radionuclide migration from the
repository.

In the UK, gas migration studies have been carried out mainly for hard rock envi-
ronments through which groundwater and gases may be able to migrate freely. This
affects the role of the Engineered Barrier System considerably, as it will have to pre-
vent radionuclide migration. The barrier system will be designed to contain short-lived
radionuclides and to limit the long-term release of long-lived radionuclides. This can
be done by controlling groundwater transportation in and around the repository, by
limiting radionuclide solubilities and by providing sorption surfaces for the radionu-
clides. The Engineered Barrier System consists of several possible elements, such as
the waste packages, backfill and seals used in the repository.

The Phased Geological Repository Concept (PGRC) is the reference UK disposal con-
cept (see for example Hicks et al., 2008). The PGRC introduces the disposal plans
for disposing L/ILW in a deep underground repository. It assumes a repository exca-
vated to a depth of 300 m - 1000 m, but does not specify the location of the facility,
nor the type of host rock. The possible disposal environments include high strength
crystalline rocks and sedimentary and evaporite rocks such as limestone, mudstone,
sandstone, clays and salt. The PGRC identifies steel or cement containers emplaced in
underground caverns, surrounded with a cementitious backfill material, as the preferred
method for waste disposal. The design of the facility depends strongly on the type of
host rock. In strong rocks large vaults maximising the available disposal volume are
preferred. These large vaults are currently expected to be approximately 300 m long,
16 m high and 16 m wide (Edmunds and Shelton, 2007).
The conditions in the repository evolve over time. During the operational phase, groundwater and gases will be removed and the repository will be kept at atmospheric pressure. The surrounding rock is at hydrostatic pressure. After repository closure, there is a large pressure gradient leading to a high initial rate of groundwater flow into the repository; groundwater starts to fill void spaces such as pore space within the backfill and the crown space. The inflowing groundwater starts the large-scale corrosion processes within the disposal vaults. The time at which groundwater enters the repository after its closure depends on the properties of the host rock and the repository design. If these are known, the gas generation rates within the repository can be estimated. In a very low-permeable host rock gases will accumulate within the repository structures; in a more permeable rock a pathway to the ground surface may become established. The migration of gases thus depends on the properties of the host rock, the repository design and the materials used within the repository.

**LUMPED MODELS**

In order to simplify gas migration modelling, the repository can be represented by a single material which combines the properties of waste packages, backfill and other materials present in the repository. Several authors have used volume-weighted averages of the backfill and waste packages as the repository material properties. In most of these, the waste packages are assumed to be impermeable and to have zero porosity, while the backfill is assumed to have values typical for a cementitious material. Bate et al. (2008) estimates an intrinsic permeability, $k$, of $4.5 \times 10^{-16}$ m$^2$, and a porosity, $\phi$, of 0.10 for the lumped material, while Hoch and Swift (2010) derive values $k = 2.0 \times 10^{-16}$ m$^2$ and $\phi = 0.08$.

A slightly different approach was adopted by Nagra (2008) who assumed the repository material consisted of cement-filled waste drums, mortar, concrete and the shotcrete lining of the tunnels. Again, the waste packages were assumed to be impermeable and to have zero porosity. The volume-weighted average for the porosity was calculated to be $\phi = 0.25$. The permeability of the repository was, however, assumed to be $k = 2.0 \times 10^{-15}$ m$^2$, a conservative estimate based on the repository containing mainly cementitious materials.

Other authors, such as Poller et al. (2009) and Senger et al. (2009), have treated the primary waste packages, concrete overpacks, crown space and backfill separately in
Figure C.1: The repository material properties will be derived by calculating the rate of water flow through a vault during steady state conditions.

their studies. A drawback of this technique is that it requires considerable computational effort. Table C.1 summarises the hydrogeological properties of the repository materials used in studies which lump the properties of all repository materials together.

<table>
<thead>
<tr>
<th>Study by</th>
<th>Permeability ($m^2$)</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bate et al. (2008)</td>
<td>$4.5 \times 10^{-16}$</td>
<td>0.10</td>
</tr>
<tr>
<td>Hoch and Swift (2010)</td>
<td>$2.0 \times 10^{-16}$</td>
<td>0.08</td>
</tr>
<tr>
<td>Nagra (2008)</td>
<td>$1.0 \times 10^{-15}$</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table C.1: Parameters used in previous studies

In this study, simulations will be carried out to derive the repository material properties. The model provides a way to measure the effective permeability of the vault by applying a pressure gradient across the vault and measuring the flow of water through it. Figure C.2 shows the vault model in more detail.

The model takes into account some of the engineering features of the repository, such as backfill and waste package materials, crown space, a low-permeability vault liner and the arrangement of waste packages within the repository. The vault consists of a $7 \times 7 \times 7$ array of waste packages (based on Edmunds and Shelton, 2007). A low-permeability permanent liner with a thickness of 30 cm and permeability of $k = 1.0 \times 10^{-19} m^2$ is used to line the vault throughout. At the top of the vault there is an empty space which is 4.95 m tall and can be filled with the cementitious backfill material, some other material such as sand or crushed rock, or left unfilled. The waste packages are taken to be 1.25 m tall and 1.5 m wide. A gap of 25 cm separates the waste packages
vertically whilst a gap of 50 cm separates them horizontally. These gaps are filled with the backfill material, which is assumed to have a permeability of $k = 1.0 \times 10^{-16}$ m$^2$. The waste packages are assumed to be impermeable.

Symmetry of the model leads to the requirement that only one quarter of the vault needs to be modelled. The mesh is shown in Figure C.3. Above and below the vault are large areas of highly permeable rock with constant pressure conditions. Zero flow boundary conditions are imposed on the sides. The material properties used in the study are shown in Table C.2.
The system is initially fully saturated with a constant pressure gradient through it. Water is injected into the bottom elements with a total rate of $4.0 \times 10^{-3}$ kg/s, and this drives flow through the vault. Once a steady state is reached, the flow rate can be used to calculate the effective permeability of the entire vault.

### RESULTS

Darcy’s law can be used to estimate fluid flow rates in porous media. The relationship between the flow rate of water, $Q_{TOT}$, and permeability, $k$, can be expressed as:

$$Q_{TOT} = -k \frac{\rho A \partial P}{\mu \partial z}$$  \hspace{1cm} (C.1)

where $\rho$ is density of water (kg/m$^3$), $A$ is the cross-sectional area through which flow occurs (m$^2$), $\mu$ is the dynamic viscosity of water (Pa·s), and $\partial P/\partial z$ is the pressure gradient driving the fluid flow (Pa/m). As the total flow rate through the vault during steady state conditions can be obtained from the TOUGH2 simulation, we can calculate the effective permeability from:

$$k = -\frac{Q_{TOT} \mu}{\rho A \frac{\partial P}{\partial z}}$$  \hspace{1cm} (C.2)

Using this method, the effective permeability for the base case is calculated to be $2.2 \times 10^{-18}$ m$^2$.

Analyses using variations of the base case were also performed. The permeabilities of the backfill, crown space and liner were changed in order to investigate which factors most affect the effective permeability of the entire vault. The permeability ranges are shown in Table C.3.
<table>
<thead>
<tr>
<th>Material</th>
<th>Permeability $(m^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Backfill</td>
<td>$1.0 \times 10^{-19} - 1.0 \times 10^{-15}$</td>
</tr>
<tr>
<td>Vault liner</td>
<td>$1.0 \times 10^{-20} - 1.0 \times 10^{-18}$</td>
</tr>
<tr>
<td>Crown space</td>
<td>$1.0 \times 10^{-17} - 1.0 \times 10^{-13}$</td>
</tr>
</tbody>
</table>

Table C.3: Variations of the base case

The results are shown in Figures C.4 and C.5. Figure C.4 shows how the effective permeability of the vault changes as the properties of backfill, crown space and liner are changed. The figure indicates that the permeability of the vault liner has the biggest impact on the effective permeability: as the permeability of the liner is increased by an order of magnitude, the effective permeability increases by nearly two orders of magnitude. The permeability of the backfill material has little effect, unless a very low permeability material is used. Similarly, the crown space has little effect on the effective permeability, even if the space is left unfilled or filled with, for example, crushed rock or gravel. The crown space permeability becomes important only when a higher permeability liner is used.

![Figure C.4: Effective permeability of the vault](image)
Figure C.5: Changes in the vault effective permeability as the properties of backfill, crown space and liner are changed

Figure C.5 shows the comparison of the results obtained using TOUGH2 and volume-weighted averages. In almost all cases averaging permeabilities leads to over-estimation of the vault effective permeability by an order of magnitude or more. This is particularly true when the crown space has got a high permeability.

**DISCUSSION**

This article presented an alternative way of estimating the effective permeability of a typical nuclear waste disposal vault. The effective permeability using the detailed model was found to be $2.2 \times 10^{-18}$ m$^2$, which is considerably lower than the permeability of the vault obtained using the volume-weighted averaging method. This may have important implications to low permeability host rocks. In these environments pressure in the vicinity of the vaults may increase considerably as gas accumulates within the vaults. More accurate gas migration studies are hence required to investigate the possible pressure increase.

The above calculations were carried out to investigate the relative importance of different design aspects to the effective permeability of the vault. The results indicate
that the permeability of the vault liner has a considerable impact upon the effective permeability. The model does not aim to provide an accurate representation of the repository, and many simplifications have been made. For example, the repository material properties do not stay constant over time; waste packages degrade and gradually become more permeable. Assuming the waste packages to be impermeable and to have zero porosity may be a valid assumption at early times, but the effective permeability of the entire vault increases over time.

The next stages of the project consider anisotropy in the effective permeability and the migration of repository gases. The effects of the repository fill materials, layout of waste packages and the arrangement of repository vaults on the gas migration will be investigated through a parametric study. The results can then be used to improve the repository design.

References


Nagra (2008). Effects of post-disposal gas generation in a repository for low- and


Appendix D

Publication 3

ILW Disposal: Modelling the Resaturation of a UK Geological Disposal Facility


Keywords: ILW disposal, resaturation, modelling.

ABSTRACT

This paper considers the resaturation process of a British ILW repository. Water flow into the vaults is modelled using a multiphase flow simulator TOUGH2. The time it takes for the vaults to fill with water is estimated paying particular attention to the effect of the repository design. The effects of the permeability of the backfill, fill material of the crown space and the properties of a low-permeability liner around the vaults are considered. The resaturation time of the vaults is found to be approximately 6.5 years. The presence of a low-permeability liner around the vaults is discovered to have a large impact on the resaturation time.

The resaturation time is calculated using a detailed model of the vault. Another, computationally less expensive, way to model the vault is to lump the vault materials together: the vault containing the waste packages is represented by one set of parameters which combines the properties of the waste packages, backfill, crown space and liner. Previous studies have taken the permeability of the 'lumped material' to be the volume-weighted average permeability of the repository materials. This paper presents
APPENDIX D. PUBLICATION 3

an alternative approach to the derivation of the effective permeability of the lumped material. The effective permeability across the vault is found to be approximately $3 \times 10^{-18}$ m$^2$. The permeability along the vault is higher, $7 \times 10^{-17}$ m$^2$, indicating that flow along the vault is faster than flow through it. The resaturation time of the repository, using the lumped permeabilities, is calculated to be 1.2 years; however it is recognised that resaturation may take considerably longer in lower permeability host rocks. It is also concluded that using volume-weighted averages may result in over-estimation of the effective permeability.

INTRODUCTION

Geological disposal is currently the preferred option for long term radioactive waste management in several countries including France, Germany, Switzerland, Sweden, Finland, the U.S., Canada and Japan. The disposal concepts developed in these countries rely on the use of both natural and engineered features to prevent the migration of radionuclides out of the repository. Some concepts, for example the French and Swiss, involve disposal in a low-permeability host rock, such as clay. Water flow through such a host rock is restricted, and the rock therefore forms the most important barrier to radionuclide migration.

Other concepts, such as the Swedish and Finnish, have been developed for fractured rocks, through which water moves more freely. These concepts reply on the Engineered Barrier System (EBS) to contain radionuclides. The EBS consists of several possible elements, such as the waste packages, backfill and seals used in the repository. It is designed to control groundwater transportation through the facility and to limit the solubility and migration of radionuclides by creating desirable chemical conditions.

The UK Disposal Concept

It has been decided that the UK low and intermediate level radioactive waste (L/ILW) will be disposed of in deep underground facilities (CoRWM, 2006). The UK generic disposal concept is called the Phased Geological Repository Concept (PGRC) (see for example Hicks et al., 2008). The PGRC introduces plans for disposing L/ILW in a repository excavated to a depth of 300 m - 1000 m, but it does not specify the location of the facility, nor the type of host rock. The possible disposal environments include high strength crystalline rocks and sedimentary and evaporite rocks such as limestone, mudstone, sandstone, clays and salt.

The PGRC identifies the preferred method for waste disposal to be waste packaged in steel or cement containers and emplaced in underground caverns which are then filled
with backfill. The repository backfill is designed so that its chemical properties prevent radionuclide migration from the vaults; a cementitious material is currently preferred. The design of the facility depends strongly on the type of host rock. The specific repository designs for different host rocks are currently under development, though the concept for a disposal facility located in fractured crystalline rock has been developed the furthest. In strong rocks large vaults which maximise the available disposal volume are preferred. These large vaults are currently expected to be approximately 300 m long, 16 m high and 16 m wide (Edmunds & Shelton, 2007).

Repository Resaturation

The conditions in the repository evolve over time. During the operational phase, inflowing groundwater is removed and the repository is kept at atmospheric pressure. The pores of the surrounding rock are filled with water. After the repository is backfilled and closed, groundwater from the rock will enter the facility and gradually fill all the air-filled space within it. The time at which groundwater enters the repository depends on the properties of the host rock and the repository design.

This paper investigates the resaturation process of the disposal vaults, with particular attention being paid to the effect of the repository materials on the resaturation time. A detailed model of a disposal vault, including the arrangement of waste packages within it, is developed.

Many modelling studies represent the repository using a single set of parameters instead of a detailed model. Bate (2008) and Nagra (2008) use volume-weighted averages to obtain the effective permeability of the repository materials. We present an alternative method of calculating the effective permeability and use the value to estimate the resaturation time of the entire repository.

VAULT RESATURATION CALCULATIONS USING A DETAILED MODEL

In this section we calculate the resaturation time of a waste disposal vault. We use a detailed model of the vault which accounts for some of the common engineered features such as waste package arrangement, backfill, crown space and a low-permeability vault liner. As the disposal vaults are several hundred meters long, the water flow into the mid-parts of the vaults will be almost two dimensional. A thin slice of the vault is therefore investigated. Furthermore, only half of the cross-section needs to be modelled due to symmetry.

Figure D.1 shows the vault model in detail. The slice of the vault considered here
Figure D.1: Vault layout for the detailed model. The figure shows the array of waste packages (in dark grey) surrounded by backfill material (in light grey), with the upper crown space (in white) and the vault sealed with a liner (in black).

Figure D.2: Mesh used to calculate the effective permeability of the vault.

consists of a $7 \times 3 \times 7$ array of waste packages (based on Edmunds & Shelton, 2007). The waste packages are 1.2 m tall, 1.5 m wide and 1.5 m deep. A gap of 30 cm separates the waste packages vertically whilst a gap of 60 cm separates them horizontally. These gaps are filled with the backfill material, which, in the base case, is assumed to have a permeability of $1.0 \times 10^{-16}$ m$^2$. The waste packages are assumed to have a very low permeability.

The top of the repository can be left unfilled, or alternatively a fill material, such as sand, gravel or backfill, can be used. This space is taken to be 4.8 m tall and, in the base case, assumed to be filled with the backfill material. A low-permeability permanent liner with a thickness of 30 cm and a base case permeability of $1.0 \times 10^{-19}$ m$^2$ is used to line the vault throughout. The vault is assumed to be located at a depth of 600 m and
surrounded by large areas of highly permeable rock with constant pressure conditions. A typical grid spacing of 30 cm is used. The properties and proportional volumes of waste packages, backfill, crown space and liner are shown in Table D.1. The mesh used in the simulations is shown in Figure D.2.

<table>
<thead>
<tr>
<th>Material</th>
<th>Permeability (m²)</th>
<th>Porosity (%)</th>
<th>Volume (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Host rock</td>
<td>$1.0 \times 10^{-14}$</td>
<td>0.3</td>
<td>n/a</td>
</tr>
<tr>
<td>Backfill</td>
<td>$1.0 \times 10^{-16}$</td>
<td>0.1</td>
<td>42</td>
</tr>
<tr>
<td>Waste packages</td>
<td>0.0</td>
<td>0.0</td>
<td>24</td>
</tr>
<tr>
<td>Vault liner</td>
<td>$1.0 \times 10^{-19}$</td>
<td>0.1</td>
<td>7</td>
</tr>
<tr>
<td>Crown space</td>
<td>$1.0 \times 10^{-16}$</td>
<td>0.1</td>
<td>27</td>
</tr>
</tbody>
</table>

Table D.1: Base case parameters

The vault is assumed to have an initial air saturation of 50 %, and the water flow from the fully saturated host rock into the vault is modelled. The simulations are performed with TOUGH2, a program developed at the Lawrence Berkeley National Laboratory for modelling multiphase flows in porous and fractured media.

Figure D.3 shows the water from the host rock entering the vault through the vault walls, ceiling and floor, and gradually filling all void space within it. The pressure gradient at the bottom of the vault is the largest, which results in the water front advancing through the floor quickest. As water flows in, air contained within the vault rises upwards in the vertical spaces between waste packages. As the space for air decreases, air compresses and dissolves in the groundwater. This behaviour is demonstrated in Figure D.4 which shows the decrease in air saturation over time in an element in the middle of the vault. The graph shows a sharp decrease in the gas saturation as the groundwater reaches the element around 6.5 years. Not all the air has, however, dissolved or escaped from the vault, and the gas saturation remains slightly elevated for several tens of years. The increase in the gas saturation around 10 years is due to the gas from areas below the element rising upwards. As the waste packages have a very low permeability, air from within them is released very slowly.

We take the resaturation time of the vault to be the time it takes for the elements within the vault to reach an average of 95 % water saturation. The resaturation time in the base case is found to be approximately 6.5 years.

The effect of the repository materials on the resaturation time was then investigated by varying the properties of the vault backfill, crown space and liner. The ranges of permeabilities studied are shown in Table D.2. These investigations were performed in order to determine the relative importance of these materials to the resaturation time.
Figure D.3: Resaturation of the disposal vault. The figure shows a sequence of gas saturation profiles taken at times 0.25 (top left corner), 1, 2, 4, 6, 8, 10 and 15 (bottom right corner) years. The gas saturation in the vault is initially 50% but decreases with time as water from the surrounding rock flows in through the walls, ceiling and floor and dissolves and displaces air.
Figure D.4: Gas saturation changes over time in the middle of the vault. Gas saturation in the vault is initially 50% but decreases sharply when water enters the element.

<table>
<thead>
<tr>
<th>Material</th>
<th>Permeability (m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Backfill</td>
<td>$1.0 \times 10^{-19} - 1.0 \times 10^{-15}$</td>
</tr>
<tr>
<td>Crown space</td>
<td>$1.0 \times 10^{-17} - 1.0 \times 10^{-13}$</td>
</tr>
<tr>
<td>Vault liner</td>
<td>$1.0 \times 10^{-20} - 1.0 \times 10^{-15}$</td>
</tr>
</tbody>
</table>

Table D.2: Variations of the base case.

Figure D.5 shows how the resaturation time depends on the permeability of the repository materials. The presence of a low-permeability liner increases the resaturation time from less than a year to 6.5 years. Figure 5 suggests that the permeability of the backfill has little effect on the resaturation behaviour unless a very low permeability material is chosen. In reality, however, the repository backfill would be unlikely to have a very low permeability. The fill material of the crown space is found to have almost no effect on the resaturation time. We therefore conclude that the vault liner is the most important material for the repository resaturation.

**REPOSITORY RESATURATION**

**Calculating the vault effective permeability**

The simulation times of two-phase flow calculations using a detailed vault model vary from several hours to several days. This section considers the approach of representing the vault with one set of material parameters in order to ease the computational load.

Several research projects have been carried out to model the repository resaturation and the two-phase flow of fluids from the repository. Authors, such as Poller et al. (2009) and Senger et al. (2009), use detailed models of the repositories in question and
model the migration of groundwater and gases through them. These models take into account the different material properties of primary waste packages, concrete overpacks, crown space and backfill. A drawback of this technique is that it requires considerable computational effort.

Instead of using the detailed repository design, a simplification can be made by representing the entire repository with a single set of material parameters. This ‘lumped’ material combines the properties of waste packages, backfill and other materials present in the repository. Several authors have used this approach in the past. Many of them calculate the lumped material properties by taking a volume-weighted average of the backfill and waste package permeabilities and porosities. The waste packages are often assumed to be impermeable and to have zero porosity, while the backfill is assumed to have values typical for a cementitious material. Bate et al. (2008) estimate an intrinsic permeability, \( k \), of \( 4.5 \times 10^{-16} \) m\(^2\), and a porosity, \( \phi \), of 0.10 for the lumped material, while Hoch and Swift (2010) derive values \( k = 2.0 \times 10^{-16} \) m\(^2\) and \( \phi = 0.08 \).

Nagra (2008) assume the repository material consists of cement-filled waste drums, mortar, concrete and a shotcrete lining of disposal tunnels. They take a volume-weighted average of the porosity, \( \phi = 0.25 \), to represent the entire repository. The permeability of the repository is assumed to be \( k = 1.0 \times 10^{-15} \) m\(^2\), which is considered to be a conservative estimate based on the repository containing mainly cementitious materials.
Model Parameters

In this paper we present an alternative method of obtaining the effective permeability of the vaults. The obtained effective permeability will be compared with the volume-weighted average value and used to calculate the resaturation time of the repository. In order to do this, simulations of water flow through the disposal vault will be performed. The same detailed vault model and material parameters as in the resaturation base case are used. The vault is initially fully saturated and a known pressure gradient is applied across it in the vertical direction. By keeping all other boundaries impermeable, we enforce flow in the vertical direction through the entire vault. Water is injected into the bottom elements with a constant rate, and the pressure difference drives flow through the vault. The simulation is allowed to run until steady state flow conditions are achieved. Once a steady state is reached, the flow rate can be used to calculate the effective permeability of the vault in the vertical direction.

The direction of the pressure gradient can then be changed to be in the horizontal direction, either across the vault or along it. The flow is again only allowed to occur in one direction, and the effective permeability in this direction is calculated.

Results

Darcy’s law can be used to estimate fluid flow rates in porous media. The relationship between the flow rate of water, $F_{TOT}$, and permeability, $k$, can be expressed as:

$$F_{TOT} = k \frac{\rho A}{\mu} \frac{\partial P}{\partial z} \tag{D.1}$$

where $\rho$ is density of water (kg/m$^3$), $A$ is the cross-sectional area through which flow occurs (m$^2$), $\mu$ is the dynamic viscosity of water (Pa s), and $\partial P/\partial z$ is the pressure gradient driving the fluid flow (Pa/m). As the total flow rate through the vault during steady state conditions can be obtained from the TOUGH2 simulation, we can rearrange Equation 1 to calculate the effective permeability of the vault. The effective permeabilities for the base case are found to be $2.7 \times 10^{-18}$ m$^2$ in the vertical direction, $2.8 \times 10^{-18}$ m$^2$ across the vault and $7.0 \times 10^{-17}$ m$^2$ along the vault. The permeability of the crown space has the largest impact upon the permeability along the vault, while the liner permeability determines the permeability across the vault in both horizontal and vertical directions.

Figure D.6 shows how the effective permeability of the vault in the vertical direction changes as the properties of backfill, liner and crown space are changed. The figure indicates that the permeability of the vault liner has the biggest impact on the effective permeability: as the permeability of the liner is varied by five orders of magnitude,
the effective permeability changes by approximately three orders of magnitude. The properties of the backfill also have a significant effect on the effective permeability. The backfill properties seem to have the largest impact when a medium-range liner permeability is used. At very low or high liner permeabilities, backfill properties have little effect. In particular, as the permeability of the liner is increased above that of the backfill, the liner allows flow of water through it more quickly than the rest of the vault. The permeability of the backfill material thus has little effect on the effective permeability. The fill material of the crown space is found to have little effect on the effective permeability, even if the space is left unfilled or filled with a higher permeability material such as crushed rock or gravel.

Figure D.7 shows the comparison of the results obtained using TOUGH2 and volume-weighted averages. In almost all cases averaging permeabilities leads to overestimation of the vault effective permeability by an order of magnitude or more. This is particularly true when the crown space has a high permeability. It is also noted that, as the liner permeability is increased, the results agree better with the volume-weighted averages. Figure D.8 shows the results of simulations in which the thickness of the liner was varied. The liner thickness has little bearing on the effective permeability beyond 10 cm.

The lumped permeability here is obtained using single-phase flow. It can, however, be applied to multi-phase problems by taking into account the relative permeabilities of the liquid and gas phases.

**Large-scale Repository Resaturation**

As already mentioned, it would not be feasible to model the entire repository in the same detail as the earlier calculations. In order to demonstrate the usefulness of the lumped approach, the resaturation of the repository was modelled using the lumped material properties. The model consists of 20 vaults which are 300 m long, 16 m high and 16 m wide. The permeability of the vaults is taken to be the effective permeability obtained in the previous section. The access tunnel is assumed to be 6 m high and 6 m wide and filled with the backfill material. The tunnels leading from the main access tunnel to the vaults are assumed to be 6 m high and 4 m wide. The vaults are separated by 50 m of host rock. The host rock is assumed to have a permeability of $1.0 \times 10^{-14} \text{ m}^2$. A part of the mesh is shown in Figure D.9. A minimum grid spacing of 2 m is used.

The repository resaturation time is now calculated to be approximately 1.2 years. This is less than the 6.5 years obtained using the detailed model, but of the same order of magnitude.

The repository resaturation time is highly dependent on the availability of water;
Figure D.6: The effect of backfill, crown space and liner material properties on the vault effective permeability. The graphs show the effective permeability on the vertical axis and the permeabilities of the backfill and crown space on the x and y axes.
Figure D.7: Effects of backfill, crown space and liner properties on the effective permeability. The volume-weighted average permeability, shown as the dashed line, is found to be much higher than the permeability derived from TOUGH2 simulations.

in very low-permeability rocks the resaturation process would be very slow. Figure D.10 shows the effect of the host rock permeability on the resaturation time. The resaturation time increases from 1.2 to over 1,000 years when the permeability of host rock is decreased from $1.0 \times 10^{-14} \text{ m}^2$ to $1.0 \times 10^{-20} \text{ m}^2$.

**CONCLUSIONS**

This paper considered the resaturation process of an ILW disposal vault. The resaturation time was calculated to be approximately 6.5 years, but it was found that the repository materials have a large impact on this value. The presence of a low-permeability liner significantly increases the resaturation time.

The paper also presented an alternative way of estimating the effective permeability of a typical nuclear waste disposal vault. The effective permeability of the vault was
Figure D.8: Effect of liner thickness on the effective permeability. The backfill, liner and crown space permeabilities are taken to be $1 \times 10^{-16} \text{ m}^2$, $1 \times 10^{-19} \text{ m}^2$ and $1 \times 10^{-16} \text{ m}^2$, as in the base case.

found to be approximately $3 \times 10^{-18} \text{ m}^2$, which is considerably lower than the permeability of the vault obtained using the volume-weighted averaging method. The results indicate that the permeability of the vault liner has a considerable impact upon the effective permeability, as does the vault backfill. The repository was found to resaturate in 1.2 years using the lumped permeabilities and assuming the host rock has high permeability. Resaturation in host rocks of very low permeability may take thousands of years.

The time at which the repository becomes fully saturated, marks the starts of the gas generation processes within the vaults; corrosion and other gas producing processes result in large quantities of gas being produced. The next stages of the project will consider the migration of repository gases out of the vault and through the host rock. The effects of the repository fill materials, layout of waste packages and the arrangement of repository vaults on the gas migration will be investigated through a parametric study.

ACKNOWLEDGEMENTS

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Figure D.9: Part of the mesh used in the repository resaturation calculations. The image shows the disposal vaults (in red) and access tunnels (in blue) surrounded by host rock.

REFERENCES

Figure D.10: The effect of the host rock permeability on the resaturation time. Resaturation may take over 1,000 years in host rocks of very low permeability.