Sealing deep site investigation boreholes: Phase 1 report



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Contact Details	AMEC, Building 150, Harwell Oxford, Didcot, Oxfordshire, OX11 0QB, United Kingdom. T +44 (0) 1635 280421, F +44 (0) 1635 280301

	Name	Signature	Date
Author(s)	C.P. Jackson		14 May 2014
	N.L. Jefferies		14 May 2014
	R. Alexander[1]		14 May 2014
	J. Smith[2]		14 May 2014
	B. Frieg[3]		14 May 2014
	I. Gauss[3]		14 May 2014
	S. Vomvoris[3]		14 May 2014
	R. Metcalfe[4]		14 May 2014
	R. Marsden[5]		14 May 2014
Reviewed by	M. Cowper		14 May 2014
Approved by	D. Lever		14 May 2014

[1] Bedrock Geosciences, [2] Galson Sciences, [3] Nagra, [4] Quintessa, [5] Schlumberger

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The report has been reviewed by Radioactive Waste Management Limited. However, references to NDA and RWMD in the text have been retained as they are appropriate for the period when this research was being performed. The views expressed and conclusions drawn in this report are those of AMEC and do not necessarily represent those of the NDA RWMD or Radioactive Waste Management Limited.

Conditions of publication

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Head of Stakeholder Engagement and Communications
Radioactive Waste Management Limited
Building 587
Curie Avenue
Harwell Oxford
Didcot
OX11 0RH
UK

email rwmdfeedback@nda.gov.uk

Executive Summary

This report presents recommendations for a programme of generic Research, Development and Demonstration (RDD) into sealing deep (i.e. >200m) site investigation boreholes.

As part of the process to obtain permission to start surface-based intrusive investigations, RWMD will be required to submit an Initial Site Evaluation (ISE) to the Environment Agency (EA). Of relevance to this study is that RWMD expect the ISE will require RWMD to provide a clear description, supported by reference to R&D and technology demonstrations, of how site investigation boreholes might be sealed. The output from the generic RDD programme into borehole sealing must be sufficient and suitable to meet Environment Agency's (EA) requirements regarding borehole sealing, in order to enable EA to issue an Environmental Permit for intrusive investigations in a timely manner. To enable this, the generic RDD programme needs to demonstrate that RWMD has developed generic approaches to sealing boreholes, and is confident that site investigation boreholes can be successfully sealed against groundwater flow and gas migration in the range of geological settings potentially relevant for a UK GDF. Once an intrusive surface-based site investigation is underway, RWMD will use the outcome from the generic R&D programme as the basis of understanding from which to develop a programme of site-specific RDD on borehole sealing.

Given the overarching objective regarding issue of the Environmental Permit, we propose the following lower level objectives for the generic RDD programme into sealing deep site investigation boreholes are:

- to advance the scientific understanding of key processes that affect seal performance;
- to understand the extent to which RWMD's illustrative borehole seal concepts are applicable to RWMD's illustrative borehole designs ('up-scaling[1]') and to the range of hydrogeological and hydrochemical environments appropriate to the different 'illustrative' geological settings in the UK;
- to identify conditions (if any) where the current RWMD seal concepts are inappropriate or where there is a significant likelihood that the seal concepts cannot be successfully implemented;
- if necessary, to develop alternative seal concepts for those conditions where current RWMD seal concepts are inappropriate or where there is a significant likelihood that the seal concepts cannot be successfully implemented.

The objectives are to be achieved from a programme that is likely to contain the following elements:

- desk-based studies, including modelling;
- laboratory experimental studies and analogue observations, to build understanding of processes and to demonstrate that the existing reference concept can be up-scaled or that viable alternatives exist;
- technology demonstration for key parts of the generic sealing systems. This would probably require demonstration experiments in overseas underground research laboratories and/or surface sites.

[1] By 'up-scaling' we mean developing the existing seal design to boreholes that are deeper and have larger diameter than the boreholes for which the seal is currently designed.

We recognise that there is an extensive knowledge base on repository sealing and on borehole sealing from other industries. A lot is known about the materials that could be used for seals and support elements and about interactions between these materials; for example, interface issues between clay and cement or steel. It is important to identify those aspects that are transferrable to borehole sealing, in order to avoid duplication of research. Some of the RDD activities that we identify in this report will therefore not require additional research. Instead, they will use the existing knowledge base and will involve developing arguments that are appropriate to the borehole sealing environment. Other significant activities will include modelling studies, engineering design and work associated with demonstrating seal emplacement.

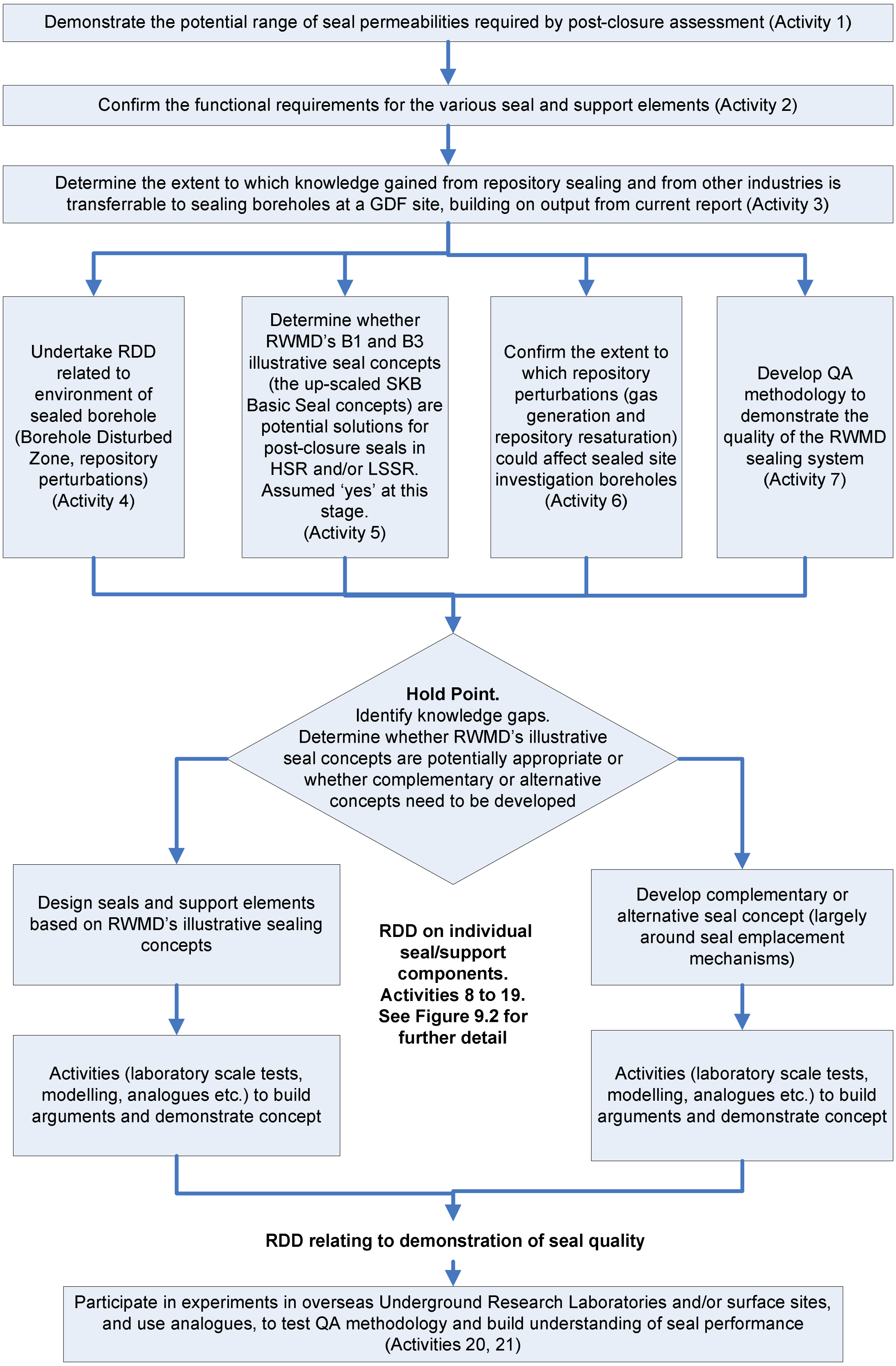
We recommend that the first requirement for borehole sealing is that the borehole should not act as a preferential pathway on a length-scale that compromises the ability of the geosphere to fulfil its principal safety functions: e.g. to '*contain the radionuclides until the radioactivity of the waste has decayed to appropriate levels*'. The objective should not be interpreted as a requirement that the borehole be sealed to the permeability of the local rock through which it was drilled. Building on this, it follows that boreholes should be sealed to the standards required by the post-closure environmental safety case. We recognise that this may only require certain formations, or parts of formations, in a borehole to be sealed by 'post-closure seals'. From a post-closure perspective, materials placed in the remaining sections of borehole are only required to provide mechanical support to the post-closure seals. However, it will also be necessary to seal boreholes to protect groundwater resources. The key issue is that the timescale over which such sealing is required will generally be much less than that required from a post-closure environmental safety case for a GDF.

We present RWMD's illustrative borehole seal concepts in the first part of this report. These form the starting point for this study, as the conclusion of participants at a previous RWMD workshop on borehole sealing concepts was that there appeared to be no major technical reasons why these sealing concepts could not be successfully adapted for the range of potentially relevant UK geologies and RWMD illustrative borehole designs. We then summarise the relevant characteristics of potentially relevant UK geological environments for a GDF. This information is presented in the context of parameterising subsequent illustrative calculations, but it also enables us to illustrate the potential envelope of conditions in which borehole seals will be placed.

The middle part of this report presents a review of the approaches taken to borehole sealing in a number of overseas radioactive waste management programmes and in the oil and gas, CO_2 storage and water resources industries. Seal materials, design, emplacement and seal longevity are all reviewed. We then present some illustrative calculations to highlight the importance of some of the issues identified through the review. Three major issues are identified from this section of the report:

- concerns that some of RWMD's illustrative seal concepts may not be appropriate in some geological environments potentially relevant to RWMD. This leads to a recommendation that the generic RDD programme contains a research strand to develop complementary or alternative seal concepts;
- a requirement to determine the post-closure performance requirements for borehole seals in a range of geological environments;
- a need to develop and test a QA methodology and demonstrate the quality of an emplaced borehole seal. This might also identify issues that would result in recommendations for borehole design.

Based on the issues identified, we conclude with recommendations for a programme of generic Research, Development and Demonstration (RDD) into sealing deep (>200m) site investigation boreholes, which are summarised in the workflow below. ‘Activities’ refer to the detailed proposed RDD programme given in Chapter 9 of this report.



Abbreviations

ALARP	As low as reasonably practicable
API	American Petroleum Institute
ASTM	American Society for Testing and Materials
BHA	Bottom hole assembly
BDZ	Borehole Damage Zone
CBL	Cement bond log
CNAP	Cyprus Natural Analogue Project
CSH	Calcium Silicon Hydrate
EA	Environment Agency
EBS	Engineered Barrier System
ECD	Equivalent circulating densities
EDZ	Excavation Disturbed Zone
EGR	Enhanced Gas Recovery
EOR	Enhanced Oil Recovery
ESC	Expansive salt-saturated concrete
GDF	Geological Disposal Facility
GRP	Glass-reinforced plastic
HLW	High Level Waste
HSR	Higher Strength Rocks
IAEA	International Atomic Energy Agency
ILW	Intermediate Level Waste
ISE	Initial Site Evaluation
ISRM	International Society for Rock Mechanics
LLW	Low Level Waste
LSSR	Lower Strength Sedimentary Rocks
LWD	Logging while drilling
MRWS	Managing Radioactive Waste Safely
MWD	Measurements taken while drilling
NA	Natural Analogue
NDA	Nuclear Decommissioning Authority
OPC	Ordinary Portland Cement
PA	Permanent Abandonment’
RDD	Research, Development and Demonstration
ROMANCON	Roman Maritime Concrete Study

RWMD	Radioactive Waste Management Directorate
RWMO	Radioactive Waste Management Organisation
SMC	Salado Mass Concrete
TIE	Third-interface echo
TDS	Total Dissolved Solid
WIPP	Waste Isolation Pilot Plant

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1 Introduction

1.1 Background

The Nuclear Decommissioning Authority (NDA) has established the Radioactive Waste Management Directorate (RWMD) to manage the delivery of geological disposal for higher activity radioactive wastes, as required under UK Government policy published in the Managing Radioactive Waste Safely (MRWS) White Paper [1]. The MRWS White Paper, published in 2008, sets out a framework for implementing geological disposal through a site selection process based on the principles of voluntarism and partnership. UK Government has recently consulted on how the siting process for a Geological Disposal Facility (GDF) could be revised and improved, while maintaining an approach based on voluntarism and partnership. Feedback is currently being reviewed.

The siting process for a GDF is currently at a generic stage; no potential sites have been identified. Section 3.9 of the recent UK Government consultation document [2] states '*There is no 'best' or 'most suitable' generic type of geology*' and '*There is a large range of potentially suitable geological settings in the UK (e.g. the Environment Agency have identified 9 potentially suitable generic settings*)'. Reference is made to [3] in the consultation document as justification for the last statement. Because the geological setting at a potential site is unknown at the current generic phase of the siting process, RWMD currently considers three illustrative geological settings (host rock formations and associated geological and hydrogeological conditions) in its development of generic disposal concepts [4].

The three illustrative geological settings for a GDF are Higher Strength Rocks (HSR), Lower Strength Sedimentary Rocks (LSSR) and evaporites. In the case of lower strength sedimentary host rocks and evaporite host rocks, the host rock will be overlain by sedimentary cover rocks. In the case of a higher strength host rock, the host rock may either extend to surface or be overlain by sedimentary cover rocks. We consider the latter case to be bounding for issues of borehole sealing in a higher strength host rock and do not consider the former case further in this report. The illustrative geological settings are discussed further in Chapter 3 and in RWMD's Geosphere Status Report [5].

The earliest phase of characterising and evaluating a site being considered for a GDF is likely to comprise of desk-based studies. If appropriate, and following issue of the necessary permits, surface-based investigations would then be undertaken at one or more sites. These surface-based investigations would include the construction and testing of a number of site investigation boreholes. Illustrative site characterisation designs are presented by RWMD in [6].

As part of the process to obtain permission to start surface-based intrusive investigations, RWMD will be required to submit an Initial Site Evaluation (ISE) to the Environment Agency (EA). Of relevance to this study is that RWMD expect the ISE will require RWMD to provide a clear description, supported by reference to R&D and technology demonstrations, of how site investigation boreholes might be sealed. The issue is related to the integrity of the geological barrier at the site, and it derives from requirements given in Environment Agency Guidance on Requirements for Authorisation for Geological Disposal Facilities on Land for Solid Radioactive Wastes [7].

This report fulfils the Scope of Work required by RWMD in their Contract Technical Specification [8]. It presents recommendations for a programme of generic Research, Development and Demonstration (RDD) on sealing deep (i.e. >200m) site investigation boreholes in the period leading up to the submission of the ISE. The output from the generic RDD programme must be sufficient and suitable to meet EA's requirements (see above) regarding borehole sealing, in order to enable EA to issue an Environmental Permit for intrusive investigations in a timely manner. To enable this, the generic RDD programme needs to demonstrate that RWMD has developed generic approaches to sealing boreholes, and is confident that site investigation boreholes can be successfully sealed against groundwater flow and gas migration in the range of geological settings potentially relevant for a UK GDF. Once an intrusive surface-based site investigation is underway, RWMD will use the outcome from the generic R&D programme as the basis of understanding from which to develop a programme of site-specific RDD on borehole sealing.

1.2 Structure of report

The remainder of this report is laid out as follows.

Chapter 2	A summary of illustrative borehole designs considered to date by RWMD, objectives for borehole sealing and illustrative borehole seal concepts. These form the starting point for this study
Chapter 3	A summary of the characteristics of potentially relevant UK geological environments. This information is presented in the context of parameterising illustrative calculations in Chapter 6, but it also enables us to illustrate the potential envelope of conditions in which seals will be placed
Chapter 4	Information on seal materials, design and emplacement. We review the approaches taken in a number of overseas radioactive waste management programmes and from the oil and gas, CO_2 storage and water resources industries
Chapter 5	The companion to Chapter 4, this time reviewing understanding of the evolution of seal properties after emplacement
Chapter 6	Additional calculations to support development of a programme of generic RDD. In this chapter, simple models are presented to highlight some of the issues identified in previous chapters
Chapter 7	Functional requirements for components of RWMD's borehole sealing systems. This presents our recommendations on the functional requirements for the different components to be used to seal boreholes at a site for a GDF
Chapter 8	Identification of key issues for RWMD's future programme of generic RDD into borehole sealing
Chapter 9	Our recommendations for a programme of RDD into sealing deep (>200m) site investigation boreholes.

Chapters 4 and 5 present a detailed review of approaches taken in a number of overseas radioactive waste management programmes and from the oil and gas, CO_2 storage and water resources industries. A discussion of the information presented is given in each of Sections 4.6 and 5.6; readers requiring only an overview could omit the earlier sections of each Chapter. Likewise, readers requiring only an overview of the additional calculations undertaken need only read Section 6.2.3 and 6.3.6. Chapters 8 and 9 identify key issues for borehole sealing and recommend a programme of RDD to address these issues. In both chapters, key supporting evidence from Chapters 4, 5 and 6 is briefly summarised to make these chapters more self-contained. The reader wishing only to understand the recommended RDD programme could therefore omit Chapters 4, 5 and 6.

1.3 Terminology used in this report

It is generally the case that more than one component is used to seal a borehole. The role of one or more of the components is to provide a low permeability in order to restrict or prevent water flow or gas through the borehole for as long as is required. In this report, we describe these components as '<u>seals</u>'. The remaining components are used to fill the remainder of the borehole and to provide mechanical support to the seals. In this report, we describe these components as '<u>supports</u>'. Elsewhere, they have been referred to as 'backfill', 'plugs' or, confusingly, 'seals'.

The process of placing materials in a borehole to prevent or restrict fluid flow is variously described as 'sealing', 'decommissioning' and 'permanent abandonment' (PA[1]). Chapter 4 gives examples of the use of these terms. 'Borehole sealing' is the terminology used by RWMD, and in this report we describe the combination of components placed in the borehole as the 'sealing system'. Borehole sealing is analogous to other closure activities in a GDF.

This report builds on earlier work for RWMD on borehole sealing, which is presented in Chapter 2. In Chapter 2, we introduce the illustrative concepts that were developed for RWMD for sealing systems in HSR, LSSR and evaporites. In this earlier work for RWMD, all materials placed were described as 'seals', even though not all have this role; in our terminology, some are 'supports'. Combinations of these 'seals' (in our terminology, seals or supports) form the illustrative sealing systems proposed by RWMD for HSR, LSSR and evaporites.

We retain the terminology of the earlier report when discussing RWMD's illustrative concepts. Likewise, in Chapters 4 and 5, which review the approaches to borehole sealing taken in a number of overseas radioactive waste management programmes and in the oil and gas, CO_2 storage and water resources industries, we retain the technology used by the various organisations and industries reviewed. From Chapter 7 onwards, when we make recommendations for a future programme of generic RDD into borehole sealing, we use the terminology of 'seals' and 'supports' to describe the various components in the sealing system.

[1] In this report, PA is an abbreviation for 'permanent abandonment'. It is not used as an abbreviation for 'Performance Assessment', which is the common use of the abbreviation in radioactive waste disposal.

2 RWMD illustrative borehole designs, objectives for borehole sealing and illustrative borehole seal concepts

2.1 Introduction

This Chapter presents a summary of RWMD's current position with regard to the design of site investigation boreholes, the preparation of these boreholes for sealing, and borehole seal concepts. All of these are at an early stage of development, as befits the current generic phase of RWMD's siting programme.

The current status of the RWMD site characterisation programme is reported in [6]. This status report gives an overview of site characterisation activities and presents RWMD's assumptions regarding a programme of surface-based borehole investigations. Subsequently, RWMD organised a workshop to consider issues affecting the design of site investigation boreholes [9]. The output from this workshop was a series of 'illustrative borehole designs', which are discussed in Section 2.2. The 'illustrative designs', which were developed by the workshop participants, are used in this report as 'working assumptions' regarding the RWMD site investigation boreholes that will require sealing. It is important to recognise that RWMD has not yet made any decisions regarding borehole design and, therefore, the RDD programme for borehole sealing must take this uncertainty into account. In Section 2.2, we also identify the key borehole design issues relevant to a generic borehole sealing RDD programme.

Section 2.3 of this report presents RWMD's stated objectives for borehole sealing. These are based on objectives developed in [10] and subsequently refined. RWMD subsequently held a workshop in 2011 to develop illustrative borehole seal concepts for a range of illustrative geological settings that are potentially suitable for a UK GDF. A report on this workshop was produced in 2011 and has recently been updated [11]. For the purposes of this report, the illustrative seal concepts described in [11] are taken to represent RWMD's current position. These illustrative seal concepts are described in Sections 2.4 and 2.5.2

2.2 RWMD illustrative borehole designs

RWMD's Site Characterisation Status report [6] presents assumptions about the scope of site characterisation activities and about some of the features of site investigation boreholes. A subsequent RWMD workshop [9] considered the factors influencing borehole design and developed illustrative borehole designs and high level drilling sequence programmes. These are described in the following sections. Illustrative borehole design figures and supporting tables are presented in Section 8 of [9]. Only boreholes drilled from surface are considered, not those drilled from underground tunnels.

2.2.1 Drilling techniques

The working assumption in this report is that both open-hole drilling and coring will be used in the construction of site investigation boreholes. The potential balance between open-hole drilling and coring boreholes is discussed in Section 7.2.5 of the Site Characterisation Status report [6]. It is concluded that '*the balance between drilling and coring is likely to be highly site- and borehole-specific*'. RWMD's illustrative borehole designs and high level drilling sequence programmes envisage that early boreholes in the site investigation process may be fully cored in order to maximise information obtained. In later boreholes, there is potential for more open hole drilling. See Section 8 of [9] for further information. Cored sections will require reaming if casing is to be placed.

The effects of drilling on the surrounding rocks are summarised in Section 4.2 of [11]. Processes that take place at the time of drilling include:

- mechanical damage and wellbore washout due to operations;
- breakout and strain due to change to the stress regime;
- chemical damage to the formation due to change in fluid chemistry, and;
- development of 'wall cake' on the borehole walls.

Together, these processes generate a Borehole Damage Zone (BDZ). In the longer term, the BDZ can develop further as a result of time-dependent stress relief effects, which can induce further breakouts.

We consider it will be possible to seal boreholes regardless of the drilling technique used. However, the RDD programme should consider the implications of different drilling techniques on borehole sealing, as the technical challenge and cost of sealing a borehole to a particular standard may be strongly influenced by the approach to construction.

The sealing concepts described in this report have the objective of sealing the wellbore, including any breakouts that form during or after drilling. There is no intention to seal the BDZ. Therefore, an understanding of the BDZ will be needed to assess flow in the disturbed zone around sealed boreholes. For example, there will be a need to understand the development and potential reversibility of the BDZ in different rock types.

The issues above are discussed in more detail in a later Section on hole quality and borehole damage (Section 4.3.6).

2.2.2 Borehole diameters and depths

The dimensions of deep boreholes are discussed in Section 7.2.4 in the Site Characterisation Status report [6]. It concludes that *'choices regarding the types of wireline logging tools, in-situ testing equipment, instrumentation and approaches to borehole sealing will be intimately connected to the choice of drilling technique and borehole diameter'*. As working assumptions for the purposes of this project, the illustrative borehole designs from [9] are used in this report. Site investigation boreholes will range from 100m to 2,000m in depth. Minimum diameter will be 6¼" (159 mm); maximum diameter will be 36" (914 mm) though in the upper part of the borehole, 26" (660 mm) would be more typical. Refer to figures in Section 8 of [9] for more details. There is a potential requirement for non-vertical boreholes during a site investigation, for example to characterise vertical or sub-vertical features at a site. Boreholes dipping at less than 45-50° are excluded from the scope of the generic RD&D programme. Demonstration of sealing such deviated boreholes could be deferred to the site-specific stage of RDD.

Reaming will be required in cored sections of borehole to allow subsequent placement of casing. Reaming will not remove the effects of breakout (it could induce new breakouts) or reduce the BDZ, as increasing borehole diameter will almost certainly increase the area of the damaged zone.

2.2.3 Casing and cementing

Issues around casing boreholes are discussed in Section 7.2.7 in the Site Characterisation Status report [6]. Illustrative casing designs are given in Section 7.2.4 of [9]. Key points from the illustrative designs are that no casing is considered necessary for HSR; in contrast, 7" casing is considered as a contingency for both LSSR and evaporites. The overburden in overlying rocks is always assumed to require casing.

Carbon steel, aluminium and glass-reinforced plastic (GRP[1])/fibreglass have all been considered by RWMD as casing materials. The RWMD assumption is that casing will be of standard American Petroleum Institute (API) carbon steel. Carbon steel, the most widely used casing material, produces the worst case environment if left in the borehole. The issues relate to the chemical interaction of steel and its corrosion products with seal materials and the generation of hydrogen gas.

RWMD's preferred approach, and base-case assumption, is that all casing is removed from the borehole prior to sealing. This approach is consistent with recommendations in a 1990 International Atomic Energy Agency (IAEA) technical report on approaches to seal boreholes, tunnels, and shafts associated with radioactive waste repositories [12]. The difficulty in removing all casing is recognised both by IAEA and RWMD[2]. Therefore, RWMD describe 'alternative' assumptions for their illustrative sealing concepts in which some casing is left in the borehole. It is important to emphasise that, even in each 'alternative assumption' (there is one for each illustrative borehole design), all casing is removed from sections of the borehole where seals are to be emplaced.

Cementation of casing was considered in [11]. This RWMD workshop emphasised the importance of achieving a high quality cement bond, as sections of cased borehole could possibly be left in-situ. However, it is important to recognise that the longevity of the cement bond will be short compared with post-closure assessment timescales.

2.2.4 Drilling flush fluid

Issues around choice of drilling flush fluid are discussed in Section 7.2.7 in the Site Characterisation Status report [6]. RWMD's proposed approach is given in Section 7.2.5 of [9] and summarised in the figures in Section 8 of [9]. The issue for borehole sealing is the invasion of drilling fluid into the formation or BDZ and the subsequent possibility that these drilling fluids could interact with seals. There will be little/no invasion in low permeability zones, so the issue could only be significant for materials placed across higher permeability zones. In such zones, the principal purpose of the material placed in the borehole will be to provide mechanical stability. As drilling fluids are unlikely to affect mechanical stability of the surrounding rocks (large-scale dissolution is not credible), any loss of drilling fluids to the formation should not be an issue. However, if the material also has a sealing function, it would be necessary to consider the impact of the drilling fluid on the permeability of the seal.

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1 An issue for GRP casing is that there is no experience of milling it out; experience of working with GRP is that tends to shatter. For GRP to be considered further, confidence will need to be built that such milling operations could be successfully performed. However, this is not a near-term RDD issue.

2 One of the reasons for inserting casings is to support unstable ground. The borehole could be prone to collapse if the casing was removed (if this was possible). Removal of casing may therefore induce significant disturbance around the borehole, which might make the sealing process more difficult.

2.3 RWMD's objectives for borehole sealing

Sealing is the final activity to be undertaken in the borehole lifecycle. RMWD has identified six objectives of sealing site investigation boreholes (Section 3.2 of [11]). The objectives are informed by the 1990 IAEA technical report [12]. A summary of this report is presented in both [10] and [11], and is not repeated here.

The RWMD objectives and subsequent text are reproduced below in italics. Our comments are shown in normal font. Note that Objectives 4, 5 and 6 are not directly relevant to the generic programme of RDD presented in this report.

Objective 1: Investigation boreholes shall be sealed with the aim of preventing them acting as preferential pathways for groundwater.

Once drilled, an investigation borehole may be used for in situ testing or for long-term monitoring utilising some form of instrumentation installed in the borehole. Whenever the completed borehole is not in use, it should be sealed to prevent the borehole acting as a preferential conduit for groundwater migration. Such migration could create disturbance to the groundwater system around the borehole and could, in the long term, act as a preferential conduit for the migration of radionuclides away from a geological disposal facility.

In the short term (i.e. when a borehole may be required for further testing or as a monitoring borehole) the borehole may be temporarily sealed using inflatable packers that can be removed to permit further scientific investigations to be carried out in the borehole. When the borehole is no longer required for scientific investigations or monitoring, it should be permanently sealed.

Implicit in the objective is that the borehole should not act as a preferential pathway on a length-scale that compromises the ability of the geosphere to fulfil its principal safety functions: e.g. to '*contain the radionuclides until the radioactivity of the waste has decayed to appropriate levels*' [5]. The objective should not be interpreted as a requirement that the borehole be sealed to the permeability of the local rock through which it was drilled.

Objective 2: Borehole seals shall be designed to be fit for purpose.

It is important to distinguish between borehole seals that are installed solely to protect the water resources in the area (water resource seals) and those that are installed to ensure that the borehole does not have a significant adverse impact on the long-term environmental safety case for the disposal facility (post-closure seals). The main differences between these two approaches to sealing investigation boreholes relates to the consideration of longevity for the seals and sealing materials. For water resource seals, it is often acceptable to partially or completely rely on steel casing in the borehole as an integral part of the seal. In contrast, it is generally regarded as preferable to avoid leaving casing in a borehole that is being sealed to post-closure standards.

The post-closure environmental safety case may only require that certain formations, or parts of formations, be sealed. These sections of the borehole would require sealing to the standards required of a post-closure seal. From a post-closure perspective, materials placed in the remaining sections of borehole are only required to provide mechanical support to the post-closure seals.

It is also necessary to seal boreholes to protect groundwater resources. For example, Environment Agency will require potential groundwater resources to be protected from adjacent saline groundwater bodies and/or from overlying anthropogenic contamination. This will require sections of the borehole to be sealed and backfilled to a standard acceptable to Environment Agency for groundwater resource protection [13]. The key issue is that the timescale over which such sealing is required will generally be much less than that required from a post-closure environmental safety case for a GDF.

Objective 3: Borehole seals shall be designed to ensure they have hydraulic properties compatible with the required performance of the geological disposal facility

The properties of the seal, the condition of the bond between the seal and the borehole walls, and the properties of the rock mass surrounding the borehole together constitute the borehole sealing system. The hydraulic properties of the sealed borehole are defined by these three component parts of the system plus any time-dependent changes that may occur to the sealing materials.

Thus, the broad objectives of the placement of borehole seals are:

- *the hydraulic conductivities of the borehole seals should be sufficiently low to ensure that the effectiveness of the geological material as an isolation barrier is not compromised;*
- *the hydraulic conductivity of the borehole sealing system should not be adversely influenced in any significant manner by the condition of the bonding between the seal and the borehole walls;*
- *the characteristics of any fractures (natural or induced by drilling) in the rock mass surrounding the boreholes should not have a significant adverse impact on the hydraulic performance of the borehole sealing system; and*
- *the properties of the sealing materials should not change significantly with time or should change slowly and predictably in such a way that the performance of the borehole sealing system will remain in compliance with the radiological protection objectives.*

The requirement for borehole seals to have hydraulic properties compatible with the required performance of the GDF means that the precise requirements for sealing a site investigation borehole will only be known after the borehole has been drilled and an understanding of the site and its post-closure performance gained. The proximity of a borehole to the potential GDF footprint, and the potential of that borehole to modify the groundwater pathway and accelerate the return of radionuclides to the biosphere, would be one aspect to consider when deciding where to locate a site investigation borehole.

Objective 4: The extent of exploratory drilling carried out in the immediate vicinity of a proposed geological disposal facility shall be kept to a minimum consistent with providing adequate characterisation of the site.

An important issue is the geometrical relationship between the exploratory boreholes and the subsequent geological disposal facility. The only sure way of ensuring that exploratory boreholes have no impact on the radiological performance of a geological disposal facility is to avoid drilling any boreholes in the vicinity of the disposal facility. Such an approach, whilst theoretically advantageous, is rarely practicable because:

- *at least some boreholes will be necessary to adequately characterise the site in order to develop engineering designs and the safety case for the disposal facility; and*
- *at the time when initial boreholes are drilled there could be some uncertainty regarding the final location of the disposal facility. Hence, there is little realistic chance of locating boreholes remote from the final disposal facility footprint.*

Objective 5: Boreholes shall be designed recognising that they will subsequently need to be sealed.

There are a number of practical approaches that can be adopted to improve the quality of the seals and reduce the impacts of exploratory boreholes on the safety case for the disposal facility. Such measures may include:

- *seeking to minimise the number of exploratory boreholes required to adequately characterise the site for a geological disposal facility, e.g. by placing greater reliability on geophysical and other non-intrusive investigations; and*
- *designing the exploratory boreholes that are required in a manner such that the ability to subsequently seal these boreholes to a high standard is not unreasonably compromised.*

Objective 6: Boreholes shall be located taking into account the potential layout of the geological disposal facility.

It is probable that at least some investigation boreholes will need to be drilled into the volume of rock that will subsequently be occupied by the disposal modules of a geological disposal facility. Indeed, it is probable that some boreholes will have been drilled before the final locations of the disposal modules have been determined.

A possible approach for a UK site could be that:

- *all investigation boreholes shall be sealed once they are no longer required;*
- *the trajectory of all investigation boreholes shall be accurately determined;*
- *any tunnel or underground excavation required as part of the construction of a geological disposal facility shall not be constructed such that any part of the tunnel or excavation is located within a defined distance (say, 10-50m) of an existing investigation borehole.*

2.4 RWMD's illustrative approach to preparing boreholes for sealing

Issues concerning boreholes are discussed in Section 7.2.8 in the Site Characterisation Status report [6]. An illustrative approach to preparing boreholes for sealing is presented in Section 5 of [11], and is described in the following Sections. We also identify the key issues that will affect the subsequent sealing of the borehole, and identify whether these are issues that should be addressed through a future programme of generic RDD.

2.4.1 Removal of installed equipment and other downhole equipment

RWMD's illustrative approach is that equipment is either removed or pushed towards the base of the borehole. If pushed to the bottom of the borehole, it is subsequently isolated by installation of seals from possibly interacting with the GDF in the future. See Section 5 of [11]. There are no issues for a generic programme of RDD into borehole sealing.

2.4.2 Reaming of borehole (including milling of casing)

RWMD's illustrative approach is that boreholes may be reamed prior to sealing, either to increase the borehole diameter to suit the seal technology or to locally or completely mill out casing to allow seals to be placed. RWMD's baseline assumption is that all casing is removed from the borehole prior to it being sealed; even under RWMD's 'alternative assumption' (see Section 2.2.3), all casing is removed from sections where seals are to be emplaced. There are no issues for a generic programme of RDD into borehole sealing. Demonstration of milling GRP casing is not an RDD issue for the near term.

2.4.3 Clean out borehole to remove debris and borehole wall cake

Cleaning out the borehole to remove debris and borehole wall cake will be undertaken as required by the sealing concept. There are no issues for a generic programme of RDD into borehole sealing.

2.4.4 Borehole condition surveys

Borehole conditions surveys are discussed in more detail in Section 4.3.6.6. At a minimum, a calliper survey will be required before the borehole is sealed, in order to determine any changes to hole dimensions that have occurred since drilling. In addition, a survey of borehole trajectory is required to ensure the location of the sealed borehole is established. The need for additional surveys will depend on the scope of testing during site characterisation, which is discussed in RWMD's Site Characterisation Status report [6]. If hydrogeological testing of lower permeability formations has not been undertaken during site characterisation, it will probably be necessary to further characterise the permeability of zones in which post-closure seals are to be placed. It may also be appropriate to determine the location of any saline transition zone before sealing, to characterise the environment in which the seals are to be placed. A generic RDD programme needs to consider these issues and come up with a solution. For example, it may be appropriate to develop a flowsheet, with supporting justification, to ensure that all necessary surveys are undertaken prior to sealing.

2.5 RWMD illustrative borehole seal concepts

2.5.1 Introduction

The description in this Section of the illustrative concepts developed for RWMD is based on [11]. Some of the RWMD illustrative seal concepts are taken from existing designs; for example, the B1 and C1 seal concepts from the SKB programme. The use of an existing design provides confidence that the seal has been demonstrated to be optimal for a particular combination of borehole diameters, depths and rock types. At the generic stage of their programme, RWMD necessarily must consider a wider range of rock types and hydrogeological/ hydrochemical conditions than considered by SKB who, from an early stage in their siting programme, only considered HSR. A key issue is to determine whether, or to what extent, the SKB concepts could be adapted to meet RWMD's requirements. The conclusion of participants at the RWMD 'sealing concepts' workshop [11] was that there appear to be no major technical reasons why these sealing concepts cannot be successfully adapted.

2.5.2 B1 seal concept

The B1 seal concept provides a post-closure seal against low permeability sections in HSR and LSSR host rocks. Where overlying casing has been removed, the B1 seal concept also provides a post-closure seal against key low permeability sections in the cover rocks. The longevity of the seal is achieved through the use of natural bentonite, which is generally stable in the natural environment. Figures in Section 8 of [9] illustrate the use of the B1 seal concept.

The B1 seal concept is based on the SKB Basis Concept, which is designed for use in 80 mm diameter boreholes up to 1,000m deep. The seal material comprises of well-fitting blocks of highly compacted bentonite, pre-dried to a water content of about 6% and then compacted to a dry density of 1,900 kg/m^3. These swell on contact with water to provide a seal against the borehole wall. To provide mechanical protection and to prevent abrasion of the blocks during seal emplacement, the bentonite blocks are contained in perforated copper tubing of 76.1 mm external diameter. The tubes have a perforation ratio of 50% with 10 mm diameter holes. On contact with water, the clay swells and migrates through the holes in the tube to form a seal against the borehole wall. The swelling pressure achieved by a bentonite seal, and hence the permeability of the seal, depends on the mass of bentonite placed, the volume of the section to be sealed and the chemistry of the groundwater. SKB calculations show their reference design seal will achieve a hydraulic conductivity of 10^{-12} ms^{-1}. Experimental proof of the SKB reference design is presented in Section 4.2.1.2.

2.5.3 B2 seal concept

The B2 seal concept has been developed by RWMD. RWMD think it is likely to be used in thick sedimentary siltstones and mudstones within cover rocks where the post-closure environmental safety case does not require the high quality long-term sealing provided by a B1 or B3 post-closure seal. It is envisaged that it will be used in conjunction with B1 and B3 seals, which are the principal long-term sealing elements. At the present time, RWMD has not defined the required longevity of the B2 seal. Our recommendations are given in Chapter 7. The design of the B2 sealing concept has not yet been completed, but the workshop [11] considered that there is potential to use a more traditional bentonite or bentonite-cement[1] grout, which can be injected/placed by pumping or dump bailer placement. Figures in Section 8 of [9] illustrate the use of the B2 seal concept in the LSSR geological environment.

2.5.4 B3 seal concept

The B3 seal concept has been developed by RWMD from the SKB reference design borehole seal. The B3 seal concept is a post-closure clay-based seal and fulfils the same purpose as the B1 seal concept. However, it is to be used in key low permeability horizons within sections of borehole where the casing has locally been milled out. Based on RWMD illustrative borehole concepts, this would imply the B3 seal concept is to be used in sedimentary cover rocks in the 'alternative' case where not all casing had been removed.

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[1] Cements are fine powders with particle sizes typically up to about 100 µm. Cement paste (or grout) is a mixture of cement particles in water. When sand is added (generally defined in the construction industry as particles up to about 5 mm) the grout becomes mortar. With larger aggregate particles added the mortar becomes concrete. Grout, mortar and concrete perform in broadly the same way but with the influence of the generally inert sand and aggregate filler becoming more dominant in either enhancing or diluting the behaviour of the cement paste matrix in mortars and concrete. In normal structural concrete, the combined sand and aggregate typically comprises 70-75% of the volume.

B3 seal concept comprises compacted bentonite in a Cu perforated tube. The diameter of the copper tubing will be controlled by the casing in the upper parts of the borehole. In the milled-out section of borehole, the difference in diameter between the copper tube and the milled and reamed borehole wall could be up to several hundred millimeters, rather than the 4 mm envisaged for the SKB reference borehole seal. In this situation, to increase the final sealing pressure exerted by the bentonite, the proposed approach is to pre-fill the section with bentonite (pumped or dumped into place) before placing the compacted bentonite in the perforated copper tube. Figures in Section 8 of [9] illustrate the use of the B3 seal concept.

2.5.5 C1 seal concept

The C1 seal concept is to be used in two situations. Firstly, where the borehole intersects flowing fracture zones within the repository host formation or cover rocks; second, in more permeable rocks within the cover sequence. In both these environments, clay-based seals would not be suitable as they would be subject to erosion by flowing groundwater[1]. The C1 seal concept does not need to have a low permeability, but it must be physically stable to provide support for the surrounding rock and overlying B1, B2 or B3 seals. The C1 seal concept is based on the SKB reference design for 'silica concrete seals', and it comprises a mixture of quartz sand and cement.

The SKB reference design includes a cement binder because sufficient mechanical stability is required at the construction phase to enable placement of the overlying borehole seal. The material has a low cement content, but is fast setting and self compacting. The cement binder is not required to be stable over the long term and will eventually be lost by leaching in groundwater. Details concerning the compositions of individual cement components, and the mineralogy of hydration products, are therefore not relevant to the long-term performance of the seal. The quartz sand remaining after the cement binder has been leached must provide long-term mechanical support to the sealing system. A range of quartz grain sizes should be used so as to provide a high density and prevent small particles from being moved by flowing groundwater. Because of concerns that leachates produced by interactions involving cement and groundwater could adversely impact the stability of bentonite in nearby B1 and B3 seals, small amounts of a 'low-pH' type of cement only should be used in C1 seals. All figures in Section 8 of [9] illustrate the use of the C1 seal concept.

2.5.6 C-SS seal concept

The C-SS seal concept is a salt-saturated cement, the design of which is derived from salt dome gas storage projects. It provides a long-term stable post-closure seal in evaporite host rocks. The salt-saturated cement mixture is emplaced in the borehole by pumping through drill pipes. Studies in Germany for gas storage projects have demonstrated that salt-saturated cement is able to crystallise within the borehole in an intimate interlocking manner such that there is no line of weakness with the borehole wall.

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1 Bentonite seals are susceptible to 'erosion' by flowing water. This places limits on the hydrogeological environments in which the seals can be used. SKB has undertaken research to define the conditions (groundwater velocities and chemistry) under which bentonite erosion will be initiated, and used this to understand the consequences on seal performance.

3 Summary of characteristics of potentially relevant UK geological environments

3.1 Introduction

To support the evaluation of borehole sealing materials and methods, this Chapter gives indicative values for geological, hydrogeological and hydrochemical parameters for potentially relevant UK geological environments. This information is presented in the context of supporting illustrative calculations, but it also enables us to illustrate the potential envelope of conditions in which seals will be placed. Key general characteristics of the different rocks that are particularly relevant for assessing borehole sealing materials and methods are:

- mechanical properties (broadly rock strength and heterogeneity of rock strength);
- hydrogeological properties (hydraulic conductivity and heterogeneity of hydraulic conductivity);
- chemical properties (broadly their degree of reactivity with respect to sealing materials, their solubility and the salinity and chemical composition of water that they contain).

Where possible, we provide generic ranges for parameters in order to provide clarity concerning the general type of rock being described. In other cases, we present parameter values used by other Radioactive Waste Management Organisations (RWMO) or typical generic values from published literature. A typical occurrence of each considered rock type is likely to have corresponding parameter values within the stated ranges. However, it is possible that there could be specific occurrences of each rock type with parameter values outside these ranges.

3.2 Generic geological environments

3.2.1 Generic Host Rock

The main characteristics of the illustrative generic host rocks that have been considered by RWMD are (reproduced from [5]):

Higher strength rocks (HSR) – These typically comprise crystalline igneous, metamorphic rocks or geologically older sedimentary rocks, where any fluid movement is predominantly through mechanical discontinuities in the rocks (fractures and faults). Granite is a good example of a rock that would fall in this category.

Lower strength sedimentary rocks (LSSR) These typically comprise geologically younger sedimentary rocks where any fluid movement is predominantly through the rock mass itself. Many types of clay are good examples of this category of rocks.

Evaporites. These comprise rocks formed from anhydrite (anhydrous calcium sulphate), halite (rock salt) or other minerals that result from the evaporation of water from water bodies containing dissolved salts.

These broad host rock groups each encompass lithologies with widely varying characteristics. Idealised process-based descriptions of the host rock environments have been developed by RWMD and used to provide a basis for statements of the overall performance that might be expected or assumed from each environment, for example in terms of a total travel time from a GDF to the surface [14].

3.2.2 Generic Cover Sequences

The sedimentary rock types that occur in a cover sequence, and the lithological heterogeneity of the sequence (i.e. degree of inter-stratification of lithologically distinct rock units), will depend upon the actual geological setting in which a given host rock occurs. Lithologies that may occur in the cover sequence include: conglomerate, sandstone, indurated shale, plastic mudstone, limestone, volcaniclastic rocks, and evaporites (principally halite or anhydrite). The characteristics of the lower-permeability cover rocks that are particularly relevant to borehole sealing are similar to those that are of concern for the host rock. Higher permeability cover rocks (e.g. sandstone aquifers) would require borehole seals appropriate for higher-permeability conditions over length scales that are considerably greater than are relevant for a host rock. For example, in a host rock, highly permeable zones (if present at all) would be narrow, probably no more than a few centimetres to metres.

3.2.3 Structures

Faults and fractures are key structures of concern when assessing borehole sealing. These structures may have different mechanical and hydrogeological properties to those of the rocks that they cut. Most faults and fractures, unless fully cemented, will be mechanically weaker than the un-deformed rock, but these structures may be either more or less hydraulically conductive than the host rock.

The characteristics and frequency of fractures in the host rock and cover sequence will depend upon the particular geological setting of a GDF. While a site will be selected so that parts of a GDF where wastes are emplaced will avoid large fracture zones, especially those that are water-conducting, such structures may still occur within the overburden or within the host rock remote from the wastes. These large faults and fracture zones may be intersected by site investigation boreholes; indeed, determining the characteristics of faults and fault rocks may be the objective of drilling a borehole. Therefore consideration needs to be given to the materials and methods that are appropriate for sealing boreholes at these intersections.

3.3 Properties of generic geological environments

3.3.1 Groundwater flow

Groundwater flow will be an important process that influences the evolution of borehole seals. Higher groundwater fluxes are likely to occur where the rock is more permeable (noting that fluxes will also depend upon the head gradient). Such relatively high-permeability rocks may be more challenging to seal than lower permeability rocks. Additionally, higher groundwater fluxes around a seal will tend to be more detrimental with respect to seal longevity than lower fluxes. For example, if a bentonite seal is suitable for such an environment, higher fluxes may lead to the erosion of bentonite seals.

Important hydrogeological properties of the rock are therefore the hydraulic conductivity and the porosity. Indicative values of these parameters for both the generic host rock types considered by RWMD and additional possible cover rocks are given in Table 3-1. It should be noted that a particular cover sequence may also include rock types that are similar to the generic host rock types.

Rock Type	Description of Flow Characteristics	Indicative Hydraulic Conductivity (ms^{-1}) and transmissivity (m^2s^{-1})	Indicative Porosity (%)	Source
HSR	Fracture-dominated flow with permeability likely to be controlled by extent and connectivity of fracture system. RWMD assumes Darcy velocity (q) through undisturbed host rock of 10^{-3} ms^{-1} to 10^{-6} ms^{-1} [14]	Hydraulic conductivity 10^{-9} to 10^{-13} ms^{-1} (over scale of tens of metres) <10^{-13} ms^{-1} (rock matrix) Fracture zones could be 10^{-5} ms^{-1} Fracture transmissivity Sparsely fractured rock (fractures typically spaced at 5 – 20m): typically 10^{-8} to 10^{-13} m^2s^{-1} Major fracture zones (clusters of flowing features might be a few m wide): typically 10^{-5} to 10^{-8} m^2s^{-1}	0.05 to 5.0 (excluding fracture zones)	[5, 15, 16, 17, 18, 19]
LSSR	Generally very low permeability - solute transport likely to be dominated by diffusion, although porous-medium flow is also possible. RWMD assume q through undisturbed host rock of $10^{-7.5}$ to $10^{-4.5}$ ms^{-1} [14]	Hydraulic conductivity 10^{-10} to 10^{-13} ms^{-1}	5 to 40	[5, 15, 20, 21]
Evaporites	Permeability extremely low or undetectable for bulk material. Interbeds may however be a source of permeability. RWMD assume specific discharge through undisturbed host rock, q, < 10^{-7} ms^{-1} [14]	Hydraulic conductivity 10^{-10} to 10^{-14} ms^{-1} (for halite - higher values correspond to strained salt) Hydraulic conductivity 10^{-8} to 10^{-13} ms^{-1} (for anhydrite) Interbeds may have much higher hydraulic conductivity, perhaps 10^{-5} ms^{-1}	0.1 to 4 (Halite - lower values correspond to intact halite, higher values correspond to strained halite) 0.5 to 5 (Anhydrite)	[5, 15, 22, 23, 24]
Permeable clastic sedimentary rocks	Permeability moderate to potentially high (minor aquifers). Flow typically through the matrix and advective mass transport likely.	Hydraulic conductivity 10^{-8} to 10^{-5} ms^{-1}	5 to 30	[5, 15]

Rock Type	Description of Flow Characteristics	Indicative Hydraulic Conductivity (ms^{-1}) and transmissivity (m^2s^{-1})	Indicative Porosity (%)	Source
Permeable limestone/ Chalk (low permeability horizons excluded; these would look more similar to some potential host rocks)	Flow may be within discrete features and the potential exists for extreme permeability (karst). In the UK, Chalk aquifers are generally considered dual porosity media	Hydraulic conductivity 10^{-6} ms^{-1} (for limestone/Chalk with primary fractures) to as high as 10^{-2} ms^{-1}) (for karst limestone) Transmissivity For English Chalk (25 and 75 percentiles for pump test data, though noting data biased towards high values) 10^{-4} to 10^{-1} m^2s^{-1}	5 to 20 (For intact limestone – karst limestone may be up to 50)	[25, 26]
Quaternary deposits	Likely to be heterogeneous, potentially on relatively short length scales. Porosity up to 0.4	10^{0} to 10^{-13} (Wide range possible reflecting heterogeneous nature of materials (gravel to clay)	25 to 60	[5, 24]

Table 3-1 Indicative hydrogeological properties of generic host rocks and possible cover rocks (note that rocks with similar properties to the generic host rocks could also occur within the cover sequence)

Groundwater flow depends not only upon the hydraulic conductivity of the rock, but also on the driving groundwater head gradients. Head gradients could vary widely, depending upon the origin of the driving force. In the UK at the kinds of depths to be investigated during site characterisation for a GDF (up to 2,000m[1]), groundwater flow is likely to be mostly driven by a combination of topographical gradients and density variations due to dissolution of rock salt. This latter process will be most important at depth within the UK's Mesozoic sedimentary basins. However, at the margins of these basins the interaction between flow systems driven by salt-dissolution and topography may be important (e.g. [27, 28]). Other factors that may influence head gradients are:

- glaciation and deglaciation, which may cause low-permeability rocks to exhibit anomalous head gradients (due to loading and unloading); and
- deeper, higher-temperature diagenetic and low-temperature metamorphic reactions, which may consume or generate free water.

These varied and inter-related factors that may influence head gradients mean that the actual gradients will be highly site-specific and also variable with respect to depth. That is, gradients may increase or decrease with respect to increasing depth over a particular depth range. However, based on published head gradients for various parts of the UK, it is suggested that gradients at most localities that might be considered to host a GDF would mostly lie up to 0.5m m^{-1}.

[1] The depth range for a GDF is 200-1,000m. However, to characterise a site it might be necessary to drill boreholes to much greater depths

3.3.2 Mechanical properties

The mechanical properties of rocks will influence strongly the deformation that could occur around boreholes (i.e. the size and shape of breakouts). Hence, the mechanical properties of the rock will also exert a strong influence on borehole sealing methods that are appropriate and the evolution of sealing materials. Indicative mechanical properties for both the generic host rock types considered by RWMD and additional possible cover rocks are given in Table 3-2. It should be noted that a particular cover sequence may also include rock types that are similar to the generic host rock types.

Rock Type	Description of Mechanical Characteristics	Indicative Uniaxial Compressive Strength (MNm^{-2})	Source
HSR	High strength	100 - 325	[29]
LSSR	Low to medium strength	1 to 100	[29]
Evaporites	Strength depends upon composition, but generally low to medium strength	5 - 110	[30]
Permeable clastic sedimentary rocks	Likely medium strength. Values for the Sherwood Sandstone Group sandstones are given here (from BGS)	30-70	[31]
Permeable limestone/chalk	Limestones will tend to be strong or very strong in international classifications but Chalk is more likely to be of medium to low strength	50 to100	[29]
Quaternary deposits	Often has very low strength so any boreholes must be cased immediately for stability	-	Not Applicable

Table 3-2 Mechanical properties of unweathered and undeformed generic host rocks and possible cover rocks (note that rocks with similar properties to the generic host rocks could also occur within the cover sequence). Weathering and / or deformation could result in lower strengths than indicated

3.3.3 Hydrochemistry

The groundwater / porewater compositions that could be encountered in the UK are variable and depend upon the particular locality considered. Within a given type of host rock and cover sequence there could be groundwater with widely variable salinity. Furthermore groundwaters /porewaters in different places (either laterally or vertically), but with similar salinities, could have considerably different chemical compositions. It is impracticable to explore explicitly the effect on borehole seal stability of all the kinds of groundwater / porewater that might be encountered. Instead, the approach taken here is to give compositions for three kinds of groundwater that are widespread in the UK (Table 3-3); most actual groundwaters will have salinities / compositions that are intermediate between them. As the issue is to consider potential salinity ranges, Table 3-3 is restricted to presentation of major ion chemistry.

- In HSR and LSSR, the water composition would most likely be Na-Cl dominated water with salinities ranging from about 75% that of seawater to brine (i.e. Total Dissolved Solid content, TDS, in the range c.20,000 mgL^{-1} to c.300,000 mgL^{-1}).

- Compared to other host rock types there would be very little water in an evaporite host rock, but there will nonetheless be some water present. This water will be halite-saturated (TDS c. 350,000 mgL^{-1}) in evaporite host rocks consisting of halite. In other kinds of host rocks (principally of anhydrite/gypsum) the salinity could be rather less, although most likely would still be NaCl-dominated brine.
- In cover rocks, the groundwater could range from brine (most likely TDS up to approximately 300,000 mgL^{-1}) to fresh water (TDS up to 1,000 mgL^{-1}). The more saline water / brine present in such a cover sequence would most likely have a Na-Cl dominated chemistry. In contrast, fresh water would most likely have Ca-HCO_3 or Na-Ca-HCO_3 dominated composition. Within a cover sequence there will probably be an increase in groundwater salinity downwards.

Determinand	Units	Brine (1)	Saline Water (2)	Ca-Na-HCO_3 fresh water (3)
		Based on Sherwood Sandstone Group Formation waters in the North Sea [32] and in the Winterborne-Kingston Borehole, Wessex Basin	Based on [27]	Based on [27]
TDS	mg/L	300,000	20,000	165
Na	mg/L	104,000	6,580	13
K	mg/L	800	102	2
Mg	mg/L	2,400	121	11
Ca	mg/L	7,100	824	33
Cl	mg/L	190,000	11,400	12
SO_4	mg/L	380	889	9
HCO_3	mg/L	24	30	124

Table 3-3 Illustrative chemical compositions of groundwater / porewater that could plausibly be encountered in the host rocks and / or cover rocks. Most water compositions that are likely to occur will be intermediate between these water types, in terms of salinity and composition

3.3.4 In-situ stress environment

The natural stress regime within the rocks that are penetrated by site characterisation boreholes has the potential to cause borehole instability, possibly leading to breakouts or detrimental relaxation. The natural stress field within the UK is variable from place to place. Furthermore, the effects of the natural stress field are not simply a function of the magnitudes of the stresses, but also:

- the orientations of the stresses with respect to heterogeneities (e.g. bedding planes) and structures (e.g. faults) within the rocks; and
- the rock strength.

Thus, the implications of natural in-situ stress for boreholes and their seals will be very site-specific. The state of stress in the UK has been reviewed recently by [33].

3.3.5 Thermal environment

Heat flow in the UK is generally relatively low. It is highest in southwest England where uranium-rich granites are close to the surface (Figure 3-1). Here, the highest heat flows are > 120 mWm^{-2} and the geothermal gradient can be 35-40℃ km^{-1} [34]. High heat production in these granites, caused in particular by radioactive decay of uranium, is the cause of the high heat flows and geothermal gradients. In contrast, the heat flow is generally lowest in sedimentary basins. The average UK geothermal gradient is 26℃ km^{-1}.

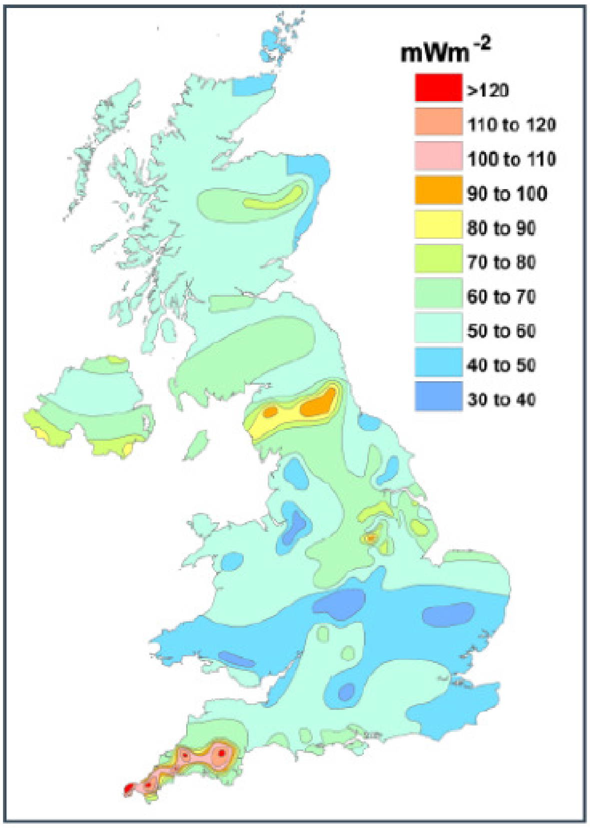


Figure 3-1 Heatflow map of the UK (after [35])

The temperature evolution of a borehole seal following emplacement will depend not only on the natural geothermal gradient at the location of the seal, but also on the thermal properties of the rock. Indicative thermal properties of the generic host rocks and rocks that may occur in the overburden are given in Table 3-4. It should be noted that rocks that are broadly similar in type to the generic host rocks may also occur in the cover sequence.

Potentially, the thermal environment could influence the evolution of borehole sealing materials. Based on the data above and on a groundwater temperature at the water table of approximately 10℃, ambient temperature at 1,000m depth is unlikely to exceed about 50℃. At 2,000m (the maximum depth considered in this report), maximum ambient temperature is likely to be approximately 90℃; average temperature at this depth is likely to be approximately 60℃. At these temperatures the chemical evolution of the sealing materials will likely be very slow, although temperature difference in the order of a few tens of degrees might significantly influence the rate at which freshly emplaced sealing materials attain their required properties (e.g. the rate at which cement cures). We also recognise that the principal materials that could be used to seal and backfill boreholes (cement and bentonite) are widely used in the near-field of many radioactive waste disposal concepts. In the near field, they may be exposed to significantly higher temperatures than in boreholes. Extensive research on the performance of clay-based and cement-based materials in these more aggressive conditions has already been undertaken.

Rock Type	Description of Thermal Characteristics	Indicative Thermal Conductivity ($Wm^{-1}K^{-1}$)	Indicative Specific Heat Capacity ($Jkg^{-1}K^{-1}$)
HSR	Unlikely to be altered at temperatures envisaged during normal evolution of a GDF	2.4 – 3.34 (from SKB)	756 – 798 (from SKB)
LSSR	May be liable to alteration at the upper end of the temperature range within a GDF	c. 2	c. 920
Evaporites	High thermal conductivity and stable at temperatures envisaged during normal evolution of a GDF. Could support higher near field temperatures	c. 5	c. 880
Permeable clastic sedimentary rocks	Within ranges for HSR and LSSR	2 – 3.34	756 – 920
Permeable limestone/chalk	Within ranges for HSR and LSSR	2 – 3.34	756 – 920
Quaternary deposits	Not applicable	Not applicable	Not applicable

Table 3-4 Illustrative thermal properties of generic host rocks and possible cover rocks (note that rocks with similar properties to the generic host rocks could also occur within the cover sequence)

3.4 Natural evolution of the geosphere

A period of one million years following closure has been used by RWMD when considering the post-closure safety case for a GDF. Significant effort has been spent internationally on identifying natural processes that may affect the evolution of the geosphere over this timescale and the contribution of those processes to GDF performance. These 'natural geosphere evolution' processes could also impact on the performance of sealed site investigation boreholes, and therefore are considered here.

Potential natural environmental changes and their possible implications for a UK GDF have been evaluated on behalf of RWMD [36]. For the majority of processes covered in this review, the possible effects on a GDF are likely to be minimal in all of the geological environments considered over the next one million years. A number of processes have been identified as having the potential to affect a GDF if circumstances are unfavourable:

- glacial erosion (relatively near surface only);

- glacial loading and unloading (which may influence groundwater heads / porewater pressures and the state of stress – see Section 3.3.4);
- permafrost (to depths of several hundred metres);
- erosion and weathering (relatively near surface only);
- changes to groundwater flow patterns (with consequent possible changes in the spatial distribution of chemically distinct water bodies, such that the salinity and composition of the water at any particular point changes over time); and
- seismicity (which is expected to be of low impact although any displacements of faults that are intersected by a borehole, such as may potentially occur during glacial loading and unloading, may be significant).

4 Seal materials, design and emplacement

4.1 Introduction

This Chapter presents information predominantly from outside the RWMD programme. We review the approaches taken by a number of RWMOs and from other industries (oil and gas; CO_2 storage; water resources) and present key issues and principles.

4.2 Experience from radioactive waste management organisations

4.2.1 Higher strength rocks (HSR)

4.2.1.1 Sealing concepts

The relevant experience for HSR draws to a large extent from investigations performed in the crystalline rocks in Sweden and Finland. An overview is given in [11] and is not repeated herein; rather the focus is on a few highlights and the additional experience accumulated since the completion of the aforementioned report.

The basic principle for developing and implementing the borehole sealing concept has been to ensure that the boreholes do not provide a flow path for groundwater and thereby do not contribute to radionuclide transport to the ground surface (or the sea floor), which has been traditionally expressed as a sealing concept that restores the hydraulic properties of the bedrock. The sealing systems designed by SKB and Posiva consist of three main components: the tight seals (main focus of this Section), the plugs for fracture zones and the plugs in the upper part of the boreholes near the surface.

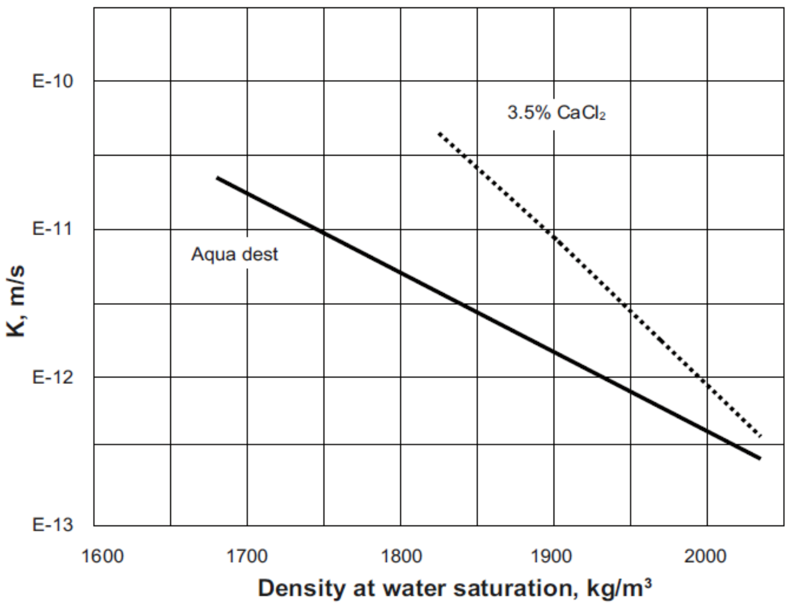


Figure 4-1 Approximate relationship between hydraulic conductivity and density for smectite-rich clay [37] for two water compositions: 3.5% $CaCl_2$ and distilled water (‘aqua dest’)

For the tight seal, the SKB design basis is that it should have a life of at least 100,000 years. The materials considered for this seal have therefore been ones with low hydraulic permeability and sufficient longevity to achieve this time scale.

The one selected and extensively studied to date has been the smectite-rich natural bentonite MX-80 (see also Section 5.2). The hydraulic and mechanical (swelling) properties of the bentonite are a function of its bulk density at maturation, which becomes the critical parameter to consider during the design and emplacement of the seals. An approximate relationship between hydraulic conductivity and bulk density for two different water compositions is shown in Figure 4-1.

Laboratory tests on MX-80 were initiated in the late 1970s and the first field tests of seal emplacement date to the Stripa international project [38]. Two series of tests were performed: first, in an approximately 95m long, 56 mm diameter sub-horizontal borehole parallel to the Buffer Mass Test drift, and; second in two sub-vertical boreholes each with a length of approximately 14m and 76 mm diameter [39]. One of the objectives of the in-situ tests was to evaluate different systems for emplacing the clay, in particular a perforated copper tube and a wire mesh. The performance of the perforated copper tube was superior and it was selected for further development.

Whereas in the Stripa tests the borehole was sealed with bentonite practically along its entire length, in the subsequent tests the design principle was modified to tightly seal those parts of the long boreholes where the rock has few fractures and a low hydraulic conductivity, and to fill the parts that intersect permeable fracture zones with physically stable material that does not need to be very tight [40, 41]. This principle is reflected in the current SKB/Posiva reference concept, as well as in concepts introduced in other programmes. The following alternatives (see also Figure 4-2) have been developed and studied to date (an overview of those is included in [11]):

1. *The Basic concept* – the boreholes are plugged with perforated copper tubes filled with highly compacted smectite-rich clay (type MX-80). A full-scale trial of this concept was conducted in a 550m deep borehole in Olkiluoto ([42], discussed below);
2. *The Container concept* – a sealed tube containing compacted smectite-rich clay is used to place the seal in the borehole. During the installation, the tube protects the seal from the borehole water. When the tube has reached the target position, the bottom is opened and the clay is pressed out. A prototype of this concept has been fabricated, but a full-scale trial has not been conducted;
3. *The Couronne concept* – a copper rod around which tightly fitting annular blocks of bentonite are fitted is placed in the borehole. The method has been tested in short boreholes in Äspö ([43] see below);
4. *The Pellet concept* – highly compacted pellets of smectite-rich clay (of type MX-80) are blown directly into the borehole. The method has been used in several different applications. It is a concept that Nagra has tested at Grimsel and used for sealing the deep investigation borehole SB4a/s at the Wellenberg site (summarised in [44]).

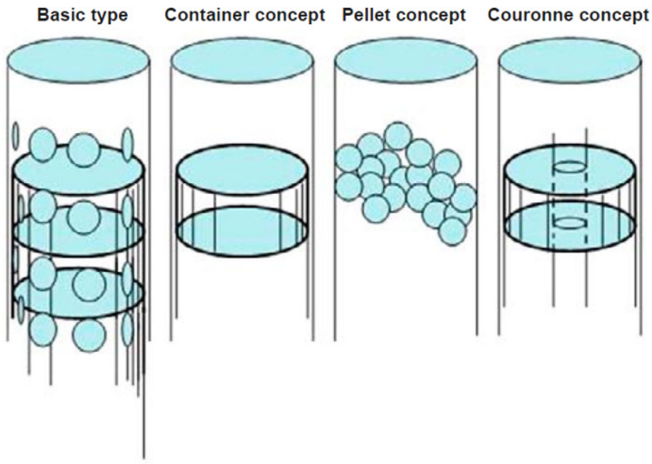


Figure 4-2 Clay plug concepts. Left: “Basic” type with dense clay blocks confined in perforated copper tubes. Second left: “Container” plug with blocks in a cylinder attached to drilling rods and released in the desired position. Third left: Dense clay pellets poured into the hole. Right: “Couronne” plug with rings of dense clay around jointed copper rods (from [45])

For the plugs for the fracture zones, the approach followed by SKB/POSIVA is to consider cement-stabilised quartz sand and/or quartzite that will provide the mechanical stability to support the rock and the clay seals above and below, and low-pH silica concrete. The proposed procedure and compositions are summarised in [11].

4.2.1.2 A full-scale test of the Basic concept

In 2005, POSIVA and SKB performed a joint field test of the concept in the approximately 550m deep investigation borehole OL-KR24 in Olkiluoto. The borehole was drilled with a diameter of 76mm along the axis of one of the future shafts. The bentonite seal had a length of 10m and was placed in the borehole section between 515m and 525m, surrounded by two 5m long low-pH quartz/concrete plugs [42]. The remainder of the borehole was backfilled with ordinary cement.

A series of tests was performed during borehole drilling to demonstrate techniques for the selective stabilisation of the borehole. The tests consisted of reaming a 2.5m long section of the borehole at the depth of 346m from 76 mm to 98 mm and applying a number of different methods to bring in the concrete to stabilise the reamed section. Difficulties encountered with the stabilisation methods, in combination with the restricted time available, meant it was not possible to conclusively complete these tests. The emplacement of the bentonite seal and the quartz/concrete plugs proceeded successfully. Some problems were encountered with the sorting of the ordinary concrete used for backfilling of the borehole, but it was concluded that these mainly were associated with small clay particles contained within the sand and such problems could be avoided in the future by proper washing of the sand.

In 2013, the shaft at the location of OL-KR24 reached the depth of 455m. The 60m long remaining section of OL-KR24 was excavated to investigate the performance of the sealing concept. The borehole was reamed to 146 mm and the sections containing the bentonite seal and the quartz/concrete plugs were overcored. The following observations have been made [46]:

- the emplacement of the upper quartz/concrete plug had a deviation of about 5m, creating an open borehole section above the bentonite seal, which was filled with water;
- the bentonite seal had swelled to the free space above, affecting the dry density at the edge of the seal; however, the dry density in the central section of the bentonite seal was about 1.67 g/cm^3; a value similar to the expected one;
- the estimated total erosion of the bentonite was about 5.6%, which is consistent with what has been estimated from laboratory experiments. Because some part of the bentonite may have been eroded during the overcoring and extraction process, the actual loss during the emplacement must have been even less;
- the perforated copper tube (visual inspection) was in direct contact with the rock, as opposed to the expectation that the bentonite would swell through the perforations and seal the contact between copper tube and rock. The authors of [46] attribute this to the good performance of the bentonite and the development of significant swelling pressures, which cracked the seams of the tubes and bent the copper to contact the rock.

The preliminary analysis of the results indicates that no significant axial transport route had remained open between the copper tube and the rock. The hydraulic conductivity investigations are expected to be completed in Spring 2014, and the final conclusions on the performance of the borehole sealing materials and emplacement methods are expected to be derived shortly thereafter.

4.2.1.3 Sealing larger diameter boreholes

The boreholes under consideration for the concepts described above vary in diameter from 56 mm to 120 mm. A first test towards applying one of these concepts to sealing larger diameter boreholes was performed at Äspö in 2009 [47]. Two existing sub-horizontal boreholes with a length of 15-20m and a diameter of 300 mm were used and the Couronne concept was applied for the seal in combination with on-site cast concrete plugs for the borehole sections in water-conducting fracture zones (see Figure 4-3). As in the other boreholes tested in HSR, these boreholes were also uncased.

In addition to the larger borehole diameter, one of the challenges of this test was the management of the inflowing water (inflow up to 30 L/minute) during the emplacement of the seals and any subsequent effects on the performance of the seal. For the former, the central tube of the Couronne concept provided a solution; for the latter, a determination could be made through a future excavation/overcoring. Note that the compaction of the bentonite blocks was such that the density at saturation was expected to be 2,017 kg/m^3, which corresponds to a hydraulic conductivity of less than 10^{-12} ms^{-1}. The emplacement of the sealing system was completed successfully and the authors [47] concluded that the performance of the seals should be expected to be very good with any degrading effect from groundwater flowing around the clay sections being minimal and localised due to the small number of water-conducting fractures in these sections. No plans for excavation of these seals have yet been made.

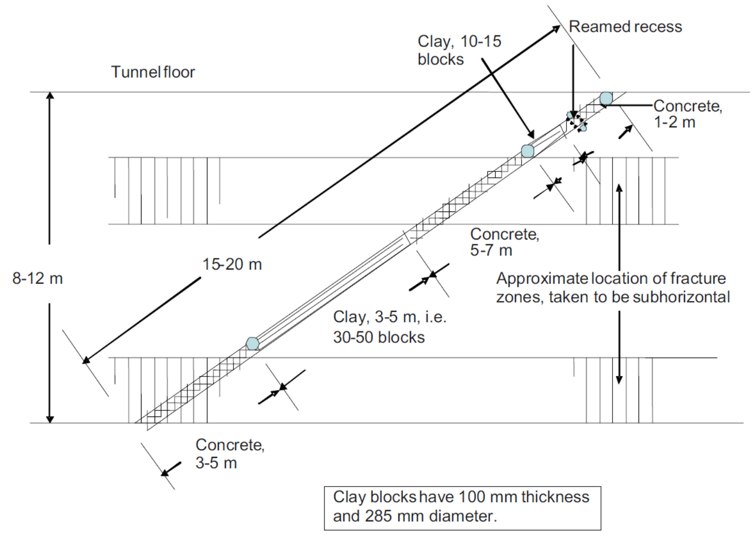


Figure 4-3 The selected sealing principle using on site cast concrete and prefabricated clay plugs (left) and the assembled clay block column ready for emplacement (right). The blocks are mounted around a central tube at the end of which a copper plate is fixed for the subsequent concrete casting ([47], courtesy of SKB)

4.2.1.4 On the requirements for borehole seals in HSR

In the majority of the field investigations, the target of borehole sealing has been to restore the rock properties. Thus, the target has been to achieve hydraulic conductivities similar to those of the low permeability sections of the borehole; these can reach values in the order of 10^{-12} m/s or lower. This approach was also used by SKB in SR-Can [48].

This requirement was further analysed in the context of the repository system Safety Case and it was concluded that, in addition to being difficult to prove in practice, such a condition would not be necessary. Thus the requirement for the seal was relaxed to a level similar to the one for the tunnel backfills and the design premise for SR-Site was defined as follows [49]:

'Boreholes must be sealed such that they do not unduly impair containment or retention properties of the repository. This is primarily achieved if the hydraulic conductivity of the borehole seal < 10^{-8} m/s, which is ensured if the swelling pressure of the seal is > 0.1 MPa. This value need not be upheld in sections where e.g. the hole passes highly transmissive zones.'

The assessment in SR-Site indicated that the design premises for sealing of the investigation boreholes could be too strict and it would be of interest to assess whether with a further relaxation, designs which would result in a higher effective axial conductivity, but more robust to control, would be sufficient.

Luterkort et al [50] revisited this premise and studied the effect of different scenarios with the groundwater flow and the mass transport/particle tracking models of the Forsmark site. Their calculations showed that, at least in the sense of 'attracting' particles, the borehole conductivity needed to be greater than 10^{-4} ms^{-1} in order to have a significant impact, and there was no or little effect when the borehole conductivity was lower than 10^{-6} ms^{-1}. They proposed the following new design premise, which has been integrated in SKB's recent RD&D plan [51]:

The resulting hydraulic conductivity over the length of the borehole shall be lower than 10^{-6} ms^{-1}.

No proposal for a new reference design for sealing of investigation boreholes is made by SKB. Preliminary studies of alternatives have been undertaken, for example sealing investigation boreholes with crushed rock that has been optimized to provide low hydraulic conductivity. However, they are not considered to be as technologically mature and proven as the current reference design. In order to change the reference design, further studies and tests would be needed.

4.2.1.5 Summary and open issues

SKB and Posiva have accumulated a substantial amount of experience with the current reference concept and on-going activities, such as the recent excavation and recovery of the system in OL-KR24, will continue to enhance this experience and highlight areas of potential future developments. For the borehole configurations considered, the emplacement densities over large sections of the bentonite have reached the targets set. Remaining issues relate primarily to technology development, for example [50]:

- improved quality control, e.g. inspection to ensure that installed components such as quartz plugs end up in the right place;
- stabilization of boreholes prior to sealing.

Finally, for the application of the reference concept to larger diameter boreholes, further studies including large-scale tests would be needed.

4.2.2 Lower strength sedimentary rocks (LSSR)

The relevant experience for LSSR draws to a large extent from investigations performed in the sedimentary rocks in Switzerland. An overview is given in [52] and [53] and is not repeated herein; rather the focus is on a few highlights.

4.2.2.1 Nagra's sealing concept

Nagra's work on borehole sealing was initiated in 1986 primarily within the low and intermediate level waste repository programme [54]. In this report the functional requirements for a borehole seal were defined as follows:

- the seal should guarantee that the groundwater flow is controlled by the surrounding rock and not the borehole; i.e. the borehole will not be a preferred flow-path or a weak zone with significantly increased hydraulic conductivity;
- the seal should ensure that if any radionuclide migration occurs through the borehole, this should not lead to any significant increase compared to the radionuclide migration through the surrounding rock;
- the seal should retain its functional properties during the construction of the repository and any changes occurring will not lead to any unacceptable increase of radionuclide release from the borehole during the post-closure phase.

A schematic view of the sealing section considered in [54] is shown in Figure 4-4. The components of the sealing section are the sealing material(s), the surrounding rock – consisting of a BDZ and the undisturbed rock – and the contact zone with the host rock. The BDZ includes the damaged zone in the immediate vicinity of the borehole wall (micro fractures shown in Figure 4-4).

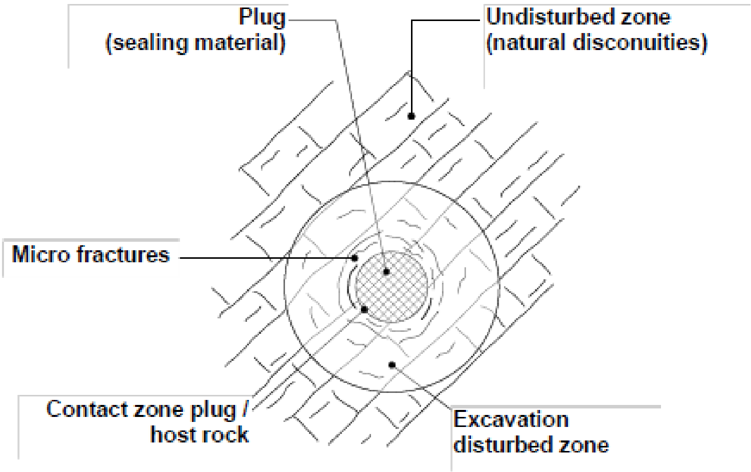


Figure 4-4 Components of a sealing section in a borehole (cross section)

The functional seal requirements defined above resulted in the following set of requirements for the materials to be used to seal boreholes at the LLW/ILW repository site.

- Mechanical strength. In the short term, the mechanical strength of the material is important for the emplacement of the material in the borehole (unless the material is brought in, in a liquid form). In the long-term, it is important for the structural integrity of the borehole.
- Deformation behaviour. The material should be ductile enough that it can survive small rock deformations without crack formation.
- Hydraulic conductivity. Should be as low as possible and in the same order of magnitude as the average conductivity of the surrounding rock. In the determination of the average hydraulic conductivity value, one should include the average conductivity of the undisturbed rock as well as the assumed conductivity for the BDZ, the latter distributed statistically around the borehole.
- Long-term stability: (i) The material should not change its chemical composition over time and no reactions with the host rock should occur. (ii) Mechanically the material should be resistant to damage caused by any environmental factors, for example groundwater flow; in particular it should be resistant to erosion. (iii) The material should be thermally stable with no irreversible changes of its properties at the expected surrounding temperature. (In most of the cases the thermal stability criterion is not relevant).
- Swelling capacity. The swelling capacity should guarantee that the void volume between the seal and the borehole wall is completely filled and consequently prevents the presence of a contact zone with hydraulic conductivity higher than that of the seal.
- Thermal conductivity. The material should have high enough thermal conductivity to allow the dissipation of any heat generated (this requirement was noted by the authors for completeness and it was recognised that it is of no importance for borehole seals).
- Workability/pumping ability: The material should be such that it can be brought into the borehole in the desired form (e.g. pre-compacted form or paste) with methods and tools available or adapted from the drilling industry.

Because no single material can satisfy all of the requirements above, Nagra developed a multi-component seal design, which is shown in Figure 4-5. The design defined two types of zones within a sealing section, each with different materials. In combination, these would meet the requirements.

- Key zones, which would correspond to more or less intact sections of the borehole; i.e. sections where the rock is intact and the magnitude and extent of the disturbed zone around the borehole is minimal.
- Intermediate zones, which surround the key zones and in which the material to provide the mechanical support for the seal zone is emplaced.

The final choice of the materials to be used in such zones depends on the host rock properties (geological, hydraulic, chemical, rock mechanical properties).

With respect to the key zones and the borehole conditions the following requirements were defined:

- their cross section should be as 'circular' as possible and should not include break-outs;
- they should be of sufficient length. The length of a key zone is determined by the length of the seal, which in turn should be determined based on the formation characteristics (i.e. it cannot be 'standardised' for all situations). The study mentions that a length of 1 - 3m could be sufficient for the geological situations considered but cautioned that such estimates can only be made after the specific geological, hydrogeological and hydrochemical conditions are known;
- the number of key zones and their locations should also be determined by the geological and hydrogeological characteristics of the formation. The study recommended to design with redundancy, for example, by including two key zones;
- the materials used in the key zones should ideally be 'natural' materials that will not interact adversely with the surrounding rock and are known to be stable for the long periods considered. Organic material should be removed from the borehole;
- the sealing materials should be in direct contact with the host rock; i.e., no casing should be present in the key zone. This requirement implies that sealing of a borehole should be considered from the very early stage of the borehole design;
- the emplacement of the seal should not cause any damage to the borehole wall;
- the hydraulic conductivity of the seal should not be higher than the hydraulic conductivity of the low permeability zones of the undisturbed rock. The consideration in the study was that in the worst case any groundwater flow would occur not through the seal but around it through the BDZ.

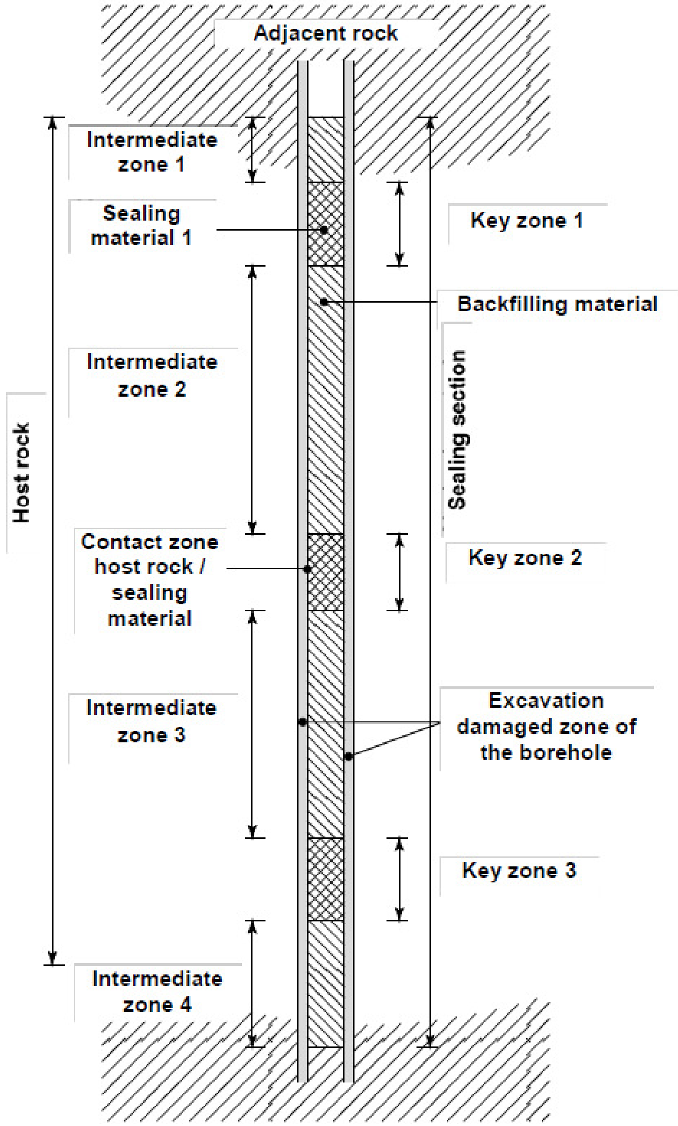


Figure 4-5 Schematic view of a multi component sealing system

The requirements for the intermediate zones were determined from their primary functions of ensuring stability and providing support for the materials in the key zone. (Note that in these zones the requirements for groundwater flow and hydraulic conductivity were less strict.) They are summarized below:

- the plug material should be primarily inorganic;
- the emplacement of the plugs in the intermediate zones should not adversely affect any of the key zones already constructed;
- the emplacement method should be a tried standard method (for example from the oil industry) and not time-consuming to implement;
- the hydraulic conductivity of the plugs should not be larger than that of the excavation disturbed zone surrounding the intermediate zone.

The functional requirements for the seals and the resulting requirements for the materials, the key zones and the intermediate zones were applied in the derivation of the sealing concept and the resulting programme for the inclined borehole SB4a/s in the Valanginian Marl of the Palfris Formation. A modification in the functional requirements for the seals in

Wellenberg SB4a/s was the extension of the 'water transport' requirement to include the transport of gas. Assuming that sealing was to be applied at the proposed repository host rock at the Wellenberg site, a sealing concept was designed to be applicable to boreholes with the following conditions:

- boreholes may contain breakouts;
- sub-horizontal;
- length of up to 500m;
- diameter of between 76 mm and 146 mm

Additional requirements for the performance of the seal were related to the expected geotechnical and hydraulic characteristics of the Palfris Formation (marl formation at Wellenberg) at the planned tunnel location. Overpressures less than 5 MPa [55] could cause hydraulic fracturing in planes of weakness; thus, the swelling pressure of the sealing material had to be limited. On the other hand it was required that the seals should reach a hydraulic conductivity in the same order of magnitude as the host rock (10^{-11} – 10^{-12} ms^{-1}).

4.2.2.2 Description of Nagra's borehole sealing system

During characterisation of the Wellenberg site in Switzerland for a low- and intermediate-level radioactive waste repository, an inclined borehole (SB4a/s) was drilled close to the planned repository area underground. Because of its location, the borehole was identified as a preferential pathway for radionuclide transport to the biosphere. Therefore it was decided that the borehole must be sealed to fulfill the criteria for the minimization of radionuclide release.

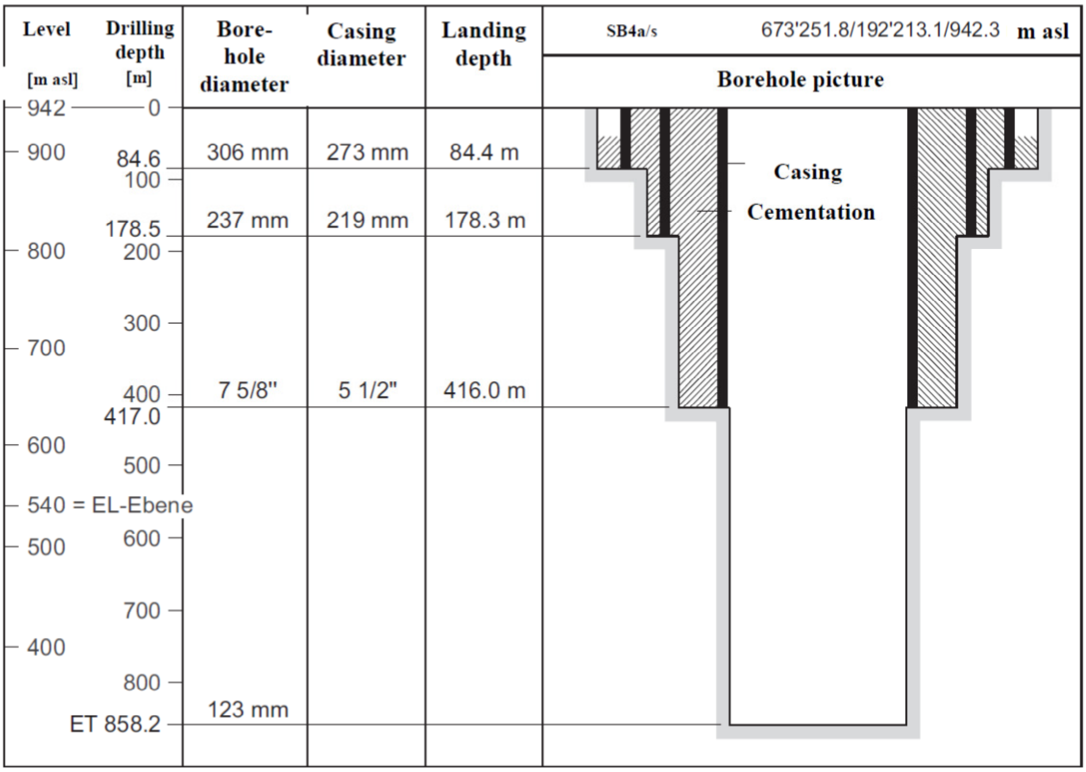


Figure 4-6 Schematic view of borehole SB4a/s

The sealing a concept was first developed based on desk studies, scoping calculations and laboratory experiments (material characterisation). The concept was then approved by the Swiss safety regulator HSK (today ENSI). Subsequently, it has been successfully applied in the field as described in detail in [53]. This approach now forms the current official Nagra concept for the sealing of boreholes drilled from the surface, and was developed in 2002.

Borehole SB4a/s was cased to a depth of 417m below ground level. The casings were fully cemented up to the surface. A schematic view of the borehole installations including the different borehole and casing diameters is given in Figure 4-6. In Figure 4-7, a profile of SB4a/s with the relevant results from the borehole investigation phase including the observed transmissivity values (m^2s^{-1}), hydraulic formation heads (m above sea level) and the encountered geology as well as the final set-up of the borehole sealing is shown. EL-N stands for the level of the planned repository.

4.2.2.3 Sealing and filling materials used in the Nagra borehole sealing concept

Laboratory experiments were carried out mainly by the Technical University of Clausthal (Germany) under the specific conditions (pressure, temperature and salinity of the water) valid for borehole SB4a/s at the Wellenberg site. These are described in [53].

Nagra developed a multi-component seal for borehole SB4a/s. The borehole seal was formed from a ~54m thick zone of barite ($BaSO_4$) underlying a ~28m thick zone of bentonite.

Barite and Quellon HD® were selected for the sealing sections for the following reasons.

- Barite ($BaSO_4$) is often used in deep drilling as an additive for the drilling fluid and for backfilling of boreholes, including for gas tight seals. It is a natural material with inert characteristics, very low solubility (the solubility product, $K_{sp} = [Ba^{2+}][SO_4^{2-}]$, in the HATCHES V20 database is $10^{-9.98}$) and high density (grain density is 4.48 Mg/m^3). The high density results in fast sedimentation, which is favourable, and compaction of the underlying sections. Barite has favourable sealant properties due to the flaky shape of its particles. It also has long-term stability: the very low solubility means that dissolution by formation fluids will be extremely slow; it is less prone to erosion by flowing groundwater than bentonite. (For the Nagra application, the size of the barite particles should not be less than 10 µm. The amount of particles bigger than 74 µm must be less than 3%.) Although more permeable than the bentonite component of the seal, the barite is considered to have a permeability approaching that of the Palfris Formation.
- Quellon HD® is a commercially available material formed from pellets of bentonite (~90%) and magnetite (~10%). The manufacturer states that Quellon HD® has '*high swelling capacity and increased density to produce waterproof sealings in deep groundwater and monitoring wells. SBF-Quellon HD annular seals are excellently detectable by geophysical logging* '[56]. The mineralogical composition is provided in Table 4-1. Before hydration, the bulk density of the Quellon-HD® pellets is 1,400 kg/m^3. After hydration in the borehole, a density of 1,880 kg/m^3 is achieved. The permeability of Quellon HD® in laboratory tests under a compaction pressure of 190 kPa (representing its compaction pressure in borehole SB4a/s) and a differential pressure of 100 kPa is about $6.3\ 10^{-19}\ m^2$ (equivalent to a hydraulic conductivity of $6.3\ 10^{-12}\ ms^{-1}$).

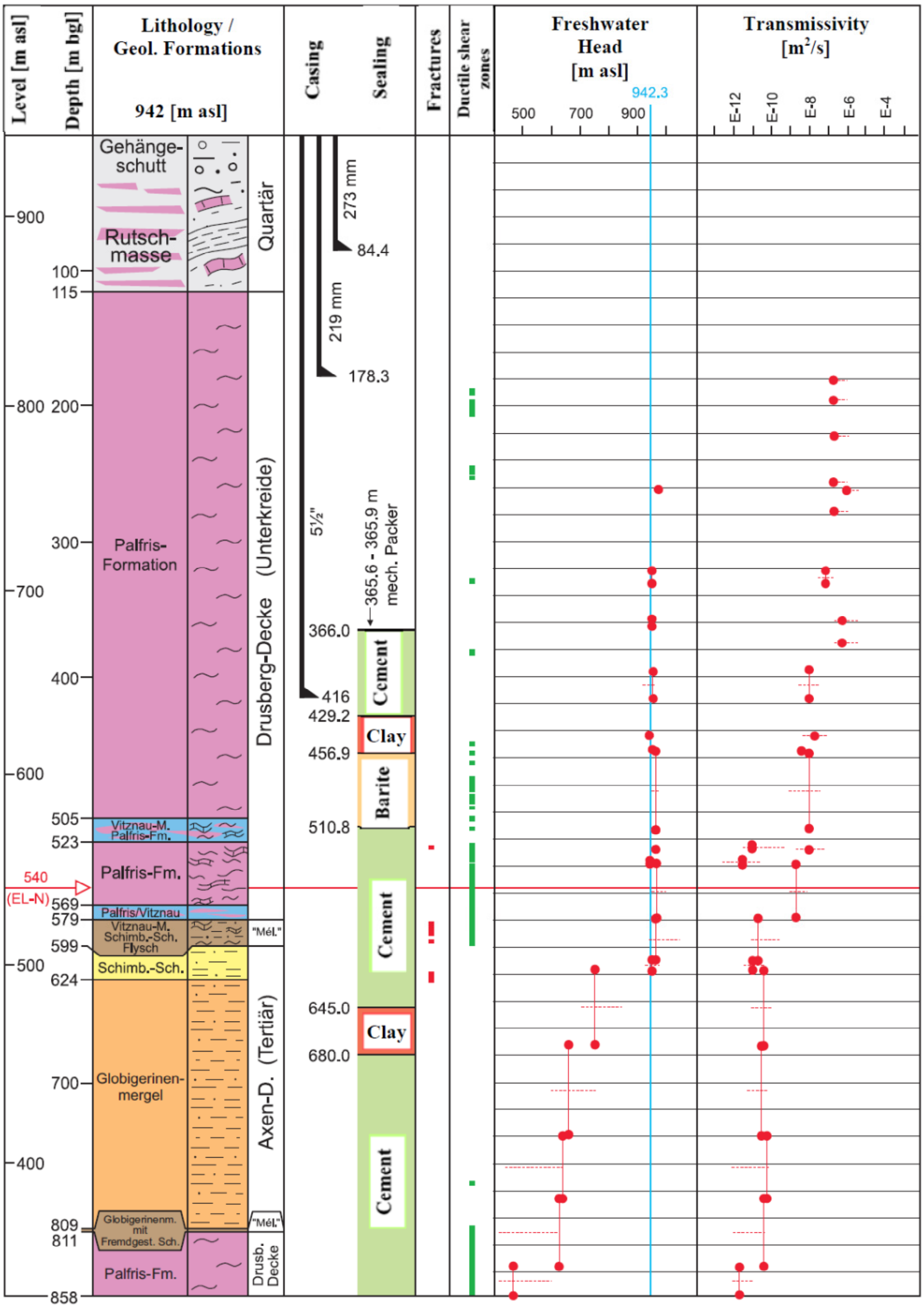


Figure 4-7 Overview of the geological profile of borehole SB4a/s which served as an example for developing the sealing concept

Table 4-1 Mineralogical composition of Quellon-HD® used for seealing Welenberg borehole SB4a/s

Phase	[Weight-%]	Determination method
Bentonite	85 – 90	Gravimetric
Magnetite	10 – 12	Gravimetric
Pyrite	1.2 – 1.3	Chemical
Silica	1 – 2	Optical
Calcite	1 – 2	Optical

Expanding cements (API Class G cements with CaO or MgO additives) were used for the intermediate zones, which surround the key zones and in which the material to provide the mechanical support for the seal zone is emplaced. Class G cements are used extensively in deep drilling. Expanding cements were chosen because, as the name implies, they expand during the hydration process (most cements shrink slightly in the course of hardening), which leads to a tight closure of the annulus of the borehole. The expanding cements were tested intensively in the laboratory before use in the borehole.

(Portland cements are used extensively in borehole sealing. A recent review for RWMD, produced by Serco in 2012 [57], gives the current status of cement materials for use as backfill, sealing and structural materials in geological disposal concepts. The reader is referred to this report for detailed information on cement systems, including: classification of Portland cements; a discussion of cement chemistry; the role of various supplementary cementing materials, admixtures and fillers in modifying cement properties and examples of cement formulations chosen for different roles in geological disposal concepts.)

As a final step of the completion a bridge plug (Type: Baker Delta 2AA) was set on top of the sealing and backfilling section inside the 5 ½”-casing from 365.9m to 365.6m along hole.

4.2.2.4 Possible alternative materials

Nagra is considering the use of sand/bentonite mixtures for engineered barriers in LLW repositories. These materials might also be appropriate for use in borehole sealing, although Nagra is not considering them in this context.

Sand/bentonite mixtures exhibit a relatively low swelling pressure compared to pure bentonite, but their mechanical properties might be an advantage in a borehole sealing context. Their hydraulic conductivity is strongly dependent on the proportion of the bentonite fraction, as is shown in Figure 4-8. Such mixtures have potential use for sealing lower permeability rocks when the proportion of bentonite is 20% or higher. This sealing material is also expected to have a favourable long-term performance, similar to that of pure bentonite, because no substantial geochemical interactions are to be expected between quartz sand and bentonite.

This type of material therefore seems promising in combining favourable mechanical properties (flexibility, resistance to bentonite erosion) with long term stability, while at the same time providing a sufficiently low permeability for certain host rock environments The material has been characterised in detail as part of the Nagra RD&D programme on sealing materials and sealing concepts for the L-ILW waste repository: Examples are the GAST experiment at the Grimsel Test Site [58] and the laboratory work of [59].

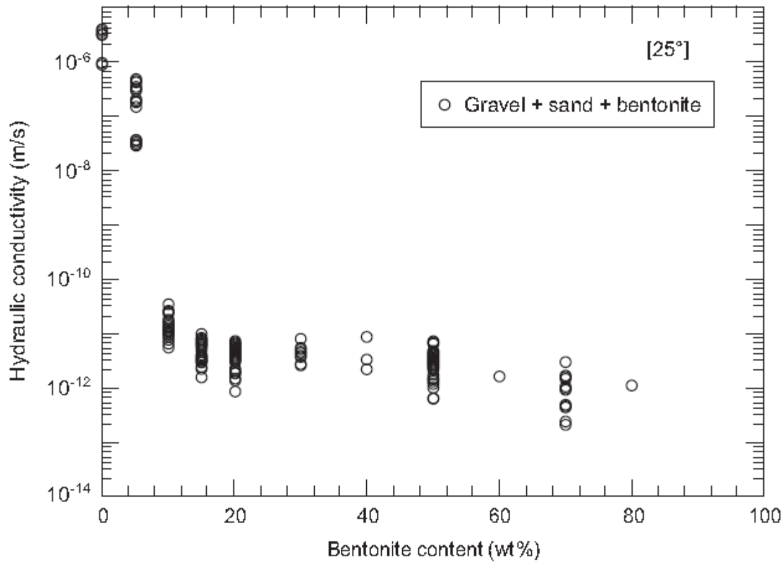


Figure 4-8 Dependence of the hydraulic conductivity of sand/bentonite mixtures on the bentonite content as described in [60]

4.2.2.5 Testing and emplacement of the sealing materials

Figure 6.9 shows the final layout of the multi component sealing system of borehole SB4a/s.

5 ½" Casing

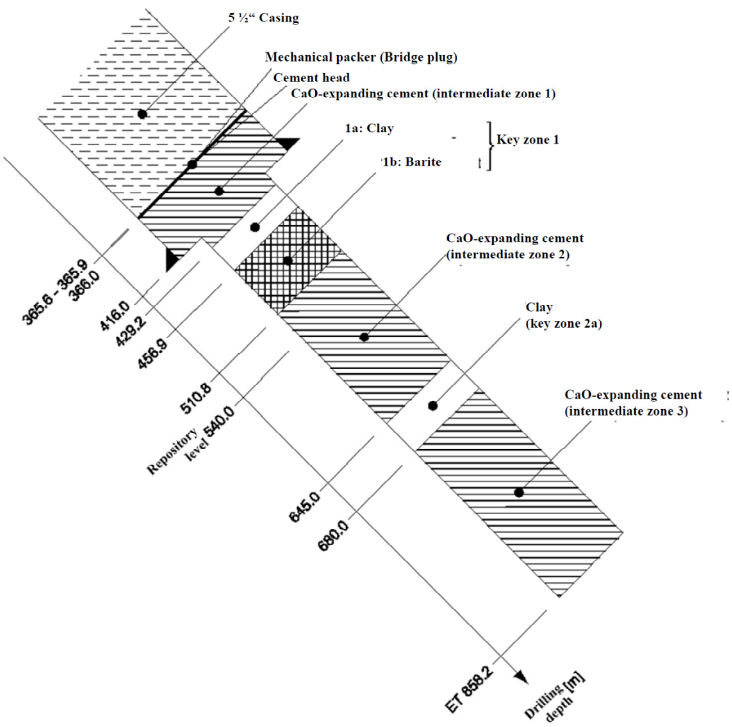


Figure 6.9 Multi component sealing system adopted in borehole SB4a/s

Sealing materials were emplaced in the borehole as suspensions ('slurries'). Issues regarding the sedimentation characteristics and filtration behaviour are described in detail in Nagra (2002). The results of the laboratory experiments for the sealing materials are summarised below.

Deep borehole cements and CaO-expanding cements

- Pumping ability. Expanding cement prepared with CaO-DORNAP[1] has a hardening time of about 7 hours. Therefore, the emplacement of expanding cement should be possible without any difficulties.
- Compressive strength. The compressive strengths of the CaO expanding cement and the normal cement for deep boreholes of class G were both within the limits required by the American Petroleum Institute.
- Swelling capacity. CaO expanding cements demonstrated a significant matrix expansion. Normal swelling cement resulted in some shrinkage.
- Hydraulic conductivity. The hydraulic conductivity of cement mixed with CaO-DORNAP was much lower than that of conventional cement. Hydraulic conductivity after 28 days was measured in the laboratory at lower than 10^{-11} ms^{-1}.

Barite and Quellon-HD®

- Pumping ability. No problem occurred while pumping the barite and the Quellon-HD®.
- Sedimentation behaviour. The main sedimentation of the barite took up to 24 hours. A suspension with a higher density tends to result in a better sealing effect.
- Sealing effect. For barite the hydraulic conductivity for a compaction pressure of 1,000 kPa was less than 10^{-8} ms^{-1}. Quellon-HD® reached less than 10^{-11} ms^{-1} with a compaction pressure of only 190 kPa.

Note that a subsequent verification test of the emplacement and/or a performance test of the seal cannot be carried out without compromising the performance of the sealing. This means that all techniques and procedures used must be tested in advance in the laboratory or in full-scale tests to guarantee that sealing meets the pre-determined requirements.

4.2.2.6 Summary and outlook for the Nagra borehole sealing concept

The Nagra concept goes back to the late 1980s and was developed finally during the 1990s. It has been accepted by the Swiss regulator and safety authorities. At the beginning, Nagra considered using an emplacement tool for the bentonite, similar to the SKB approach. However, the potential for major breakouts and possible borehole stability problems led Nagra to discard this emplacement concept. Nagra instead preferred a sealing system that used robust procedures with a low tendency of failure. In particular, pumped placement is a well-established technique.

The sealing concepts discussed in the previous paragraphs have been developed making certain assumptions regarding the rock properties encountered during the period when Nagra was investigating the Wellenberg site as a potential location for a Low Level Waste repository. From a hydrogeological point of view, the host rock targeted by the reconnaissance borehole SB4a/s is considered as a fractured medium with an extremely

[1] CaO-DORNAP is the name of the additive that was used in the cement mixture for expansion (Dornaper Hartbranntkalk Porokalk B, RWK Kalk AG Hönnetal)

low permeability matrix. For practical purposes it is assumed that groundwater is conducted exclusively by brittle features such as fault zones and fractures.

Since the activities on the sealing of boreholes as described above, Nagra's programme has changed significantly as a consequence of the implementation of the Sectoral Plan. Nagra are currently in Stage 2 of the Sectoral Plan, which concludes with the selection of at least two sites for investigation. Consequently, at the current time there is no need to further develop concepts for borehole sealing in the light of the differences between the currently proposed potential host rocks (Opalinus Clay for HLW and/or LLW, Brown Dogger and Effingen Marls for LLW) and the selected host rock at the time of the Wellenberg investigations (Valanginian Marl of the Palfris formation).

The future requirements for sealing are expected to be fairly similar to the current requirements. The impact of the much lower permeability of Opalinus Clay (several orders of magnitude lower than that of the Valanginian Marl) needs to be evaluated, particularly in light of the understanding that diffusion is the dominant transport process in Opalinus Clay. In any event, minimising the number of boreholes penetrating the host rock at the repository site is clearly desirable.

4.2.3 Evaporites

4.2.3.1 Introduction

Work on sealing boreholes in evaporites has been undertaken both for the German radioactive waste disposal programme and at the Waste Isolation Pilot Plant (WIPP) in the USA. In addition, there is substantial work on sealing salt caverns, for example for gas storage projects.

Much of the work in the German programme on materials and concept development is carried out by DBE on behalf of the Federal Office for Radiation Protection (Bundesamt für Strahlenschutz, BfS), which regards the information as its intellectual property. As a result, very little published information is available. The summary in Section 4.2.3.2 is drawn from one publicly available BfS report and several conference papers. Work on sealing of boreholes in evaporites has also been undertaken. Experience from the WIPP programme is summarised in Section 4.2.3.3. This work has already been extensively reported for RWMD in [11].

4.2.3.2 German programme

The repository projects at Morsleben, Gorleben and Asse are all set in evaporites and require exploration boreholes to be sealed. The backfilling material is based on magnesia (MgO) cement, although the exact recipe varies according to the specific requirements placed on the seal (e.g. permeability, temperature and operational constraints). The seal performs two functions: mechanical stabilisation and prevention of seepage.

At Morsleben, exploration boreholes are up to hundreds of metres in length and between 46 mm and 183 mm in diameter [61]. The mechanical requirements of the hardened grout material are:

- E-modulus of 5-25 GPa
- Uniaxial compressive strength of >15 MPa
- Uniaxial tensile strength of >1 MPa
- K-value (hydraulic conductivity) of $<10^{-10}$ ms^{-1}

In addition, the material must not shrink during setting, and pouring of the material during emplacement must not cause the rock to fracture.

The material must be temperature-resistant to 80 °C, and the adiabatic temperature maximum following the reaction process during setting should be <60 °C. The heat released during setting must not cause any significant thermal stresses within the borehole walls. There are also rheological requirements, because the flow properties of the material strongly influence both the effectiveness of the seal and the ease with which it can be emplaced. These requirements include the ability to pump the material and a working time of >2 hours at 25 °C.

The grout recipe used at Morsleben, developed by K-UTEC/ERCOSPLAN in collaboration with the BfS, is a mixture of the cementing material (MgO), a rock salt or rock flour aggregate, and $MgCl_2$ solution. The dry components comprise:

- 10 wt % MgO
- 55 wt % finely milled anhydrite powder
- 30 wt % fine rock salt (grain size 130-400 μm)
- 5 wt % slate flour.

Each kilogram of dry material is mixed with 260-265 mL 3.4M $MgCl_2$ solution. The components are fully mixed in a mixing tank before emplacement.

The grout is mixed according to written instructions and must comply with the specified recipe to within 3%. It is then emplaced using a high-pressure pumping system, but pressures must not exceed the fracturing pressure of the rock (about 10 MPa in halite and 5 MPa in potash). Mixing and pumping equipment is mobile and should allow for a variable throughput up to $5m^3$ per hour. Ensuring safe operations is a key part of emplacement, including adequate rock stability and ventilation.

Horizontal boreholes or those with shallow inclines are closed with a packer before sealing (removed after complete solidification of the seal), and an inflation or air pressure hose is used to reach the end of the borehole. Neither of these is required for steeply inclined boreholes. If a borehole to be filled contains brine, a filling material with a greater specific gravity should be used in order to displace it.

A more experimental discussion of materials that could be used for backfilling and sealing in German evaporites is presented in a DBE Technology 2007 conference paper [62] which describes a ‘family’ of materials involving the mixing of Mg-bearing salts with salt solutions. The reference recipe for this study consisted of kieserite ($MgSO_4.H_2O$) as the binding component, halite (NaCl) aggregate, a small amount of silica fume and a saturated NaCl solution. This mixture is characterised by a high fluidity, which enables transport through pipes over long distances. The mixture hardens as a result of salt hydrate crystallisation, and shows the opposite swelling progression to cement-based materials. Cement-based materials swell initially before shrinking, whereas the material tested underwent a short period of shrinking during the early hardening phase, before swelling to reach a strain of 0.33% after 21 days when the measurement was stopped. A review of the structural reliability of salt rock geotechnical barriers (focusing on shaft and drift seals, but also relevant to borehole seals) is provided in a second DBE Technology conference paper [63].

The German Repository Research Centre, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS), has also undertaken research into borehole sealing in evaporites, although its recent work is not readily available. GRS conducted experiments during the 1990s in the Asse mine into the sealing of disposal boreholes (60 cm diameter, 15m deep) using a backfill of crushed salt below a salt concrete seal [64]. The main focus of the experiments was the long-term behaviour of the salt backfill, and this is discussed in Section 5.2.3.

4.2.3.3 WIPP

The Waste Isolation Pilot Plant (WIPP) repository is constructed in bedded halite within the Salado Formation of southeastern New Mexico, USA. Sealing of site investigation boreholes or wellbores, typically ~6-8 inches in diameter, has been considered since its conceptualization, for example through the Borehole Plugging programme [65]. Early studies suggested that borehole seals with effective permeabilities greater than 10^{-11} m^2 (i.e. unplugged or with extremely permeable plugs) would still only result in calculated doses to maximally exposed individuals less than 0.001 % of the natural background radiation dose [66], well below that required for bounding safety assessments.

Freshwater grout, saltwater grout and salt concrete reference materials were developed and tested in shallow boreholes in the floor of repository-depth excavations in salt at the WIPP site during the 1980s [67] as part of the Plugging and Sealing Program. Objectives of the programme included assessment of long-term geochemical and mechanical stability of candidate seal materials. The materials were emplaced during the early-mid 1980s and samples were periodically recovered, and their mechanical and chemical integrity tested, for up to 6 years afterwards.

The freshwater grout (BCT-IFF) consisted of Class H cement (a Portland cement with low tricalcium aluminate content), fly ash to reduce heat evolution during early hydration and for durability, and calcium sulphate to form expansive phases. This material was designed for minimum permeability and maximum durability, and was shown to be compatible with anhydrite, but not with halite. The saltwater grout (BCT-IF) was developed by adding enough fine granulated salt to the freshwater mixture to saturate the mixing water. Laboratory tests proved that this improved the bond at the grout-halite host rock interface by preventing dissolution of the host rock by the freshwater. Salt also has set-retarding and water-reducing benefits. Seals made of this material were emplaced by pumping it into vertical test holes.

The expansive salt-saturated concrete (ESC) contained an expansive admixture (marketed by Master Builders as Chem Comp III), and large amounts of calcium sulphate and calcium aluminosulphate to promote early chemical expansion. Sufficient sodium chloride to saturate the mixing water was added to the dry components prior to mixing. Other components were chosen to produce specific desired effects: coarse-ground oil well cement to increase the working time (because it hydrates slowly), fly ash to improve workability and cohesion, and sodium citrate to retard the calcium sulphate. Aggregate, necessary to reduce early heat evolution, improve physical properties and reduce cost, was sourced locally. The resulting mixture had a working time of over 3 hours, and a setting time of over 9 hours, and represented a refinement of the saltwater grout to meet additional requirements for a borehole sealing material. It was emplaced into both vertical boreholes (by free fall or tremie placement) and horizontal boreholes using a concrete pump.

The components of the saltwater grout and salt-saturated concrete references are presented in Table 4-2 [67].

Component	Proportion (% of total by mass)	
	Saltwater grout (BCT-IF)	Salt cement (ESC)
Portland Cement, Class H	48.3	9.03
Chem Comp III (expansive admixture)	-	6.02
Class C fly ash	16.2	5.10
Calcium sulphate (plaster)	5.7	1.80
Fine aggregate	-	34.11
Coarse aggregate	-	34.58
Salt (NaCl)	7.9	2.50
Dispersant	0.78	-
Defoamer	0.02	0.21
Sodium citrate	-	0.11
Water	21.1	6.60

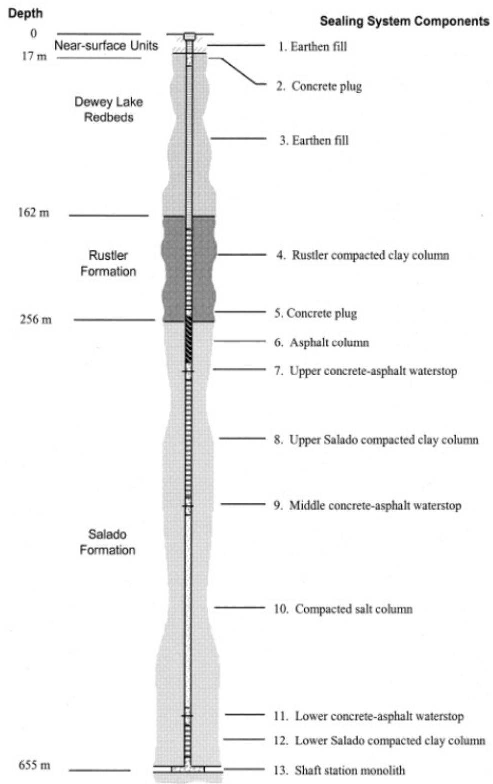
Table 4-2 Components of saltwater grout and salt concrete reference materials

During the early 1990s, a new salt-saturated concrete, Salado Mass Concrete (SMC), was developed, tested and refined for use as a seal component, particularly designed for use in large monoliths [68]. This used clean sodium chloride rather than the host rock salt, as the latter contains non-halite salts as well as other minerals which could decrease workability and strength.

Halite, in the form of crushed salt, was considered as a natural plug because of its "sealing and healing" properties. However, it was noted that such a plug would be vulnerable to groundwater inflow during the early healing phase, which could be controlled by bracketing with low-permeability grout plugs to provide initial protection [69].

This combination of salt and salt concrete is employed in the current design for a shaft sealing system for four shafts (3.5-6.1 m) at the WIPP (Figure 4-9) [70]. Although not specifically designed for sealing site investigation boreholes, there are likely to be overlapping principles. Large-scale emplacement tests, such as the Bell Canyon Test in the late 1970s (emplaced in a 4,000+ ft borehole through oil-bearing formations), showed that no great length of plug is necessary for it to fulfil its sealing function: a length on the order of 50-100 feet in any given formation is adequate [69]. This would allow secondary seals (such as clays for radionuclide absorption) to be emplaced in addition to the primary seals.

Figure 4-9 WIPP shaft sealing system



4.3 Experience from oil and gas industry

4.3.1 Introduction

Within the oil and gas industry there are numerous standards and guidelines for the permanent abandonment (PA) of exploration and development wells. Those developed by regulatory authorities and state organizations vary from country-to-country, and even from state-to-state in the USA and Canada [e.g., 71, 72, 73, 74, 75, 76, 77]. Other national guidelines have been developed by industry organizations operating in those countries, such as the API, UK Oil and Gas, and NORSOK [78, 79, 80, 81]. In addition, most major oil companies also have their own internal standards for PA, which they employ throughout their international operations to ensure (as a minimum) that all local requirements and industry recommendations are met, and that they are usually exceed by some considerable margin.

Guidelines and requirements exist for PA of any onshore boreholes in the UK [82, 83]. UK industry must also conform to the more detailed and stringent requirements and guidelines for onshore and offshore oil and gas wells that are provided by Oil and Gas UK in their Guidelines for the Suspension and Abandonment of Wells [51] and their Guidelines on Qualification of Materials for the Suspension and Abandonment of Wells [80]. NORSOK [81] provides equivalent guidelines for Norway.

The UK industry guidelines and requirements were the outcomes of a technical study of PA operations conducted by UK Oil and Gas [84] against a background of some major PA campaigns that started pre-2007. They apply both to wells that have already encountered movable fluids and any wells located where movable fluids may exist in the future, and they also comply with national regulations, which in the case of the UK are the Offshore Installations and Wells Design and Construction (DCR) Regulations [85].

4.3.2 Permanent abandonment objectives

In essence, PA operations for oil and gas wells seek to achieve, on a permanent basis:

- the prevention of the escape of any fluids from the well;
- the restoration of seals between permeable intervals (or that provided by a caprock) to conditions at least as effective as the original in situ formations (i.e., restoring the caprock);
- protection of freshwater-bearing (groundwater) zones [78];
- to reduce risk to as low as is reasonably practicable (ALARP), with allowance being made [80, 85] for:
  - deterioration of some components of the well over time;
  - the possible recovery of formation fluids to virgin pressures (or to higher pressures due to natural processes);
  - possible exposure of the well to higher induced formation pressures due to other nearby field operations (i.e., water injection for enhanced recovery).

In terms of longevity, it is realistic to say that the oil and gas industry's view is that a permanent seal is something that will perform for at least 1000 years as engineered, and beyond that timescale any borehole collapse and the associated natural movements of the formation surrounding the PA (usually sedimentary formations in the case of oil and gas drilling) that may occur will be sufficient to maintain the seal to the reservoir.

4.3.3 Plug/barrier materials

The main requirements for PA and plugging materials of oil and gas wells are that they:

- have very low permeability, to prevent flow of fluids through the barrier;
- possess long-lasting isolation characteristics, and do not deteriorate over time;
- are resistant to any downhole fluids and gases (including CO_2, hydrocarbons, H_2S etc.);
- exhibit mechanical behaviour (strength and stiffness) that will accommodate loads and potential changes to the pressure and temperature environments that they might be exposed to;
- are non-shrinking and able to bond to the formations and any casing:
  - to prevent any flow past the barrier/plug, or flow in any casing annulus;
  - to prevent change in position of the barrier in the well.

Cement is currently used as the prime material for PA of most oil and gas wells, but most regulations do not preclude the use of other materials so long as they conform to the above requirements and those specified for cement plugs. Compacted bentonite is widely used in some PA operations in the US.

One specially formulated mix of bentonite and barite with silica sand (known as SANDABAND®) is being increasingly used for plugging and PA of oil and gas wells. Although a small proportion (say 5-6%) of bentonite in cement was used in early PA activities, the industry does not now tend to use such mixtures. This is because the benefits of cement are its strength, whilst that of bentonite is the ability to swell and self-seal. Rather than offering a combination of these characteristics, the mixing of the two components tends to compromise them. (A hydrated cement will impede the swelling, and clay-contamination will impede cement strength and bond).

Indeed, this exact topic was discussed at the recent Q4-2013 meeting of the Drilling Engineering Association (Europe) DEA(e) (on 5th/ 6th December 2013, at Teddington, UK), in a special event on 'Well Abandonment' attended by major oil companies and oilfield service companies operating in the North Sea. The concern expressed by both the operating companies and service companies attending the meeting was that mixing cement and bentonite into a single barrier might reduce effort and rig-time, but will compromise the way each sealing material works rather than offering the best of both worlds. In addition, there were concerns expressed about the potential for density segregation and particle aggregation during placement, leading to a heterogeneous barrier.

Hence, if needed, the oil industry generally employs separate cement plugs and bentonite plugs, each being optimized for its own particular performance, thereby maintaining optimum performance and material characteristics of the separate materials.

The industry does utilize a range of special cements to achieve characteristics such as thermal stability, high flexibility, self-sealing and low density (for example, [86, 87, 88]), but these are not extensively used in PA. Many have complex chemistries and compositions (including polymers) that may make them unsuited to PA for post-closure seals at the site of a GDF. Nevertheless the information on these may still be of some interest to RWMD, if only to eliminate them as candidate materials. There also are other special resistant cements (for example, [89] for CO_2 storage applications). See also Sections 4.4 and 5.4.

For an oil and gas industry perspective on seal properties and their qualification, see Section 5.3.

4.3.3.1 Cements

The bulk of the cementing and well plugging for PA performed in the oil and gas industry uses API Oilwell Cement, otherwise known as Portland cement. This is placed as a slurry, so (due to the requirement that it be highly pumpable in relatively narrow annuli over long hole sections) oilfield cements are much thinner and exhibit far less strength than cements or concretes used for construction. Various additives are used to control density, setting time, strength and flow properties, and special additives are often used to reduce the occurrence of annular gas flow. After being pumped downhole the cement slurry is allowed to solidify, typically for 12 to 24 hours to achieve a compressive strength in excess of 5,000 psi (34.5 MPa)[1], before additional drilling or well activity resume.

Neat cement (i.e., with no additives to modify its setting time or rheological properties) is also used, as are advanced oilfield cements that achieve higher set-cement compressive strengths by blending a variety of particle sizes and types (sometimes including pozzolans) with less water than conventional mixtures of Portland cement, water and chemical additives.

Additional of silica flour (typically 30-40% of the dry cement), in order to prevent the formation of undesirable dicalcium silicate (leading to strength retrogression and

[1] Though not for salt – salt saturated cements, which take longer to set and build modest strength

increased porosity in the hardened cement), is normally only used in the mix where static downhole temperatures are in excess of 110℃.

4.3.3.2 Solid clays

The oil industry (particularly in the USA and California, and particularly ChevronTexaco) began to investigate the use of solid bentonite for plugging wells in 2000, realising that clay plugs might offer distinct advantages over cement in a number of ways:

- bentonite possesses an ability to deform, swell and self-seal in situations where:
  - there might be ground movements;
  - there are tectonic activities;
  - casings left in hole have corroded;
- bentonite may impede or eliminate gas migration.

The first pilots [90, 91], conducted under the guidance of the Californian State authorities (DOGGR) and involving vertical wells to 3,500ft (but mostly shallower than 2,000ft) proved very successful and led to the establishment of the first State regulations for the use of bentonite for plugging oil and gas wells [74]. These requirements are that:

- sodium bentonite is used, exhibiting a minimum specific gravity of 2.0 (dry)/1.5 (hydrated);
- pH is between 6 and 12;
- no additives are to be used. That is, no additional materials (such as higher density iron minerals) should be added to the bentonite to modify its placement or sealing properties;
- the bentonite must be placed in compressed form (typically pellets, nodules or bars [92]), and not as powder;
- wellbores must be flushed and circulated with at least one hole-volume of fresh water prior to the placement of bentonite, to remove contamination that might prevent the bentonite from hydrating and swelling;
- fresh water is maintained over a bentonite plug for a minimum of 24 hours to ensure full hydration.

The first pilot outside of the USA was in Australia in 2002 [93], to a depth of 2,100 ft in which a plug exceeding 200 ft in length was successfully placed inside a 5½" casing.

Since then, a large number of wells (certainly in excess of 1,000, but nearly all vertical and mostly shallower than 2,000 ft) have been plugged and abandoned across the US, and to a much lesser extent elsewhere, using a highly compressed, pelleted bentonite termed 'Zonite' that, when hydrated, is less permeable than hardened cement. These plugs (usually exceeding 100 ft) are typically placed inside casing that will remain in the hole for the PA, but they are also placed in open-hole sections from which casing has been cut and pulled. Occasionally, Zonite is also used to seal the annulus behind large sections of casing that have been heavily perforated and cavity-washed, but it is not used in squeeze jobs (see Section 4.3.5.1).

Interest in using such compacted bentonite materials beyond just the US and a few other countries continues, and is reported in [94, 95]. However, it is likely that for deeper and deviated well PA applications and those offshore, such materials will be largely passed over in favour of new and emerging pumpable solutions (e.g., SANDABAND®) that:

- offer similar sealing and non-setting benefits as compacted bentonite;
- are much easier to emplace across a wider range of trajectories, depths and well geometries (see Sections 4.3.5.1 and 4.3.5.2);
- have no setting times;
- hence offer rig-site time savings versus both cement and compacted bentonite, with associated cost savings.

4.3.3.3 SANDABAND®

Since 2010 the oil industry, particularly in the North Sea, has been using a solid material termed SANDABAND® [96] as a frequent alternative to cement slurry for use in temporary suspension/well plugging and in PA applications.

SANDABAND® is a 'dry' mix of bentonite clay and barite plus up to 75% quartz sand, with just some water and a very small quantity of viscosifiers and dispersant that together give the mix Bingham-plastic characteristics. This means it behaves as a liquid when pumped but then returns immediately to a solid when at rest. The first use of SANDABAND® in 2010 was for the PA of UK well 25/8-17, which was achieved by pumping a 290m long plug as the permanent primary barrier for the reservoir.

As well as being pumpable, other key attractions of SANDABAND® [94, 95, 96] are:

- it is an incompressible, gas-tight material;
- it yields and deforms if its strength is exceeded;
- it is non-shrinking, non-fracturing, non-segregating;
- it is able to self-heal and reshape resulting in no leakages in micro-annuli or similar pathways;
- it is thermodynamically stable, chemically inert, and does not suffer from contamination;
- it is stable to downhole fluids like H_2S, CO_2, and hydrocarbons;
- unlike cement, there are no losses of any liquid phase to the formation, or premature curing;
- like a slurry, it spreads laterally and finds its own level inside uncased boreholes.

Despite these attributes, SANDABAND® seals are frequently used in conjunction with shallower cement plugs, to provide additional mechanical support in the PA.

4.3.4 PA design

The numerous standards and guidelines for PA of oil and gas wells, coming from regulatory authorities, industry organizations and the oil companies themselves (see Section 4.3.1) offer a multitude of options for the design of the final seal configurations. In the UK, a minimum of two permanent barriers to vertical flow in the well are required [79].

It is widely recognised that cemented steel casing does not constitute an everlasting barrier to lateral flow into or out of the well, due to the likelihood of it corroding and leaking, but also due to the potential (if not initially, but in the future) of an incomplete or compromised cement sheath [79, 81]. Likewise, the presence of a corroded casing or impaired cement sheath will ultimately render the PA ineffective in terms of preventing some vertical flow. However, in most oil and gas PAs, at least some steel casing will be left in the hole simply due to the huge costs and logistics needed to remove it. Also, if a formation has its own internal vertical communication, establishing a complete barrier by replacing all casing through that formation with an impermeable plug will not achieve anything in terms of providing a seal.

Thus a frequent requirement of PA in oil and gas wells (if not from regional legislation or guidelines, then from internal PA standards of the oil companies themselves) is that when casing will remain in the hole then at least one plug (usually cement) is placed across the entire wellbore and across any annulus casing sections that might remain in a well from which upper sections have been pulled [97]. Lengths of plug vary, but 100 ft of cement is usually specified as a minimum requirement. Where separate isolation of several permeable zones is required, several such plugs (straddling each interval) may be necessary.

When casings cannot be pulled and they need to be removed from the hole, they are milled. In the majority of these cases the procedure is to mill a window through all casing strings, which may require several trips to expose all annuli and the formation. Cement or other pumpable material is then pumped in to the milled hole section, against the exposed formation (see Section 4.3.5.1).

Figure 4-10 Cement plug set across milled window to provide primary barrier to flow

Note also that by and large the oil and gas industry does not place the primary seals for any permeable intervals across the intervals themselves, recognising that:

- cementing such intervals can be difficult where there is any flow (natural, or induced by surging and swabbing the hole during tripping etc.) as it can lead to channelling through the barrier before it sets or is fully placed;
- permeable intervals can also be ‘thief-zones’, so can take up seal material that is intended for the hole itself. As many of the calculations for seal design are based on volumetrics, and the top of the emplaced seal is only tagged later to ensure it is of sufficient extent, this can mean an underestimation of material that needs to be pumped;
- the ultimate objective of the seals is to prevent vertical cross-flow between permeable zones, so it matters little if an isolated permeable zone is not sealed at the borehole as it will have its own internal communication. Hence failing to seal the zone at the

borehole will not change that communication, and all that will be achieved is a thin column of impermeable material in an otherwise permeable rock mass. Instead, it is more important to achieve vertical isolation of such intervals from ones below and above, so that vertical cross-flow between them is prevented.

Hence, primary seals in the permeable intervals themselves they are not deemed reliable enough to be the primary seal for oil and gas wells. Instead, the primary barrier to prevent flow from a permeable zone is achieved by placing a plug (usually cement) across the entire wellbore immediately above any permeable interval, and across the bottom of any casing sections that might remain in a well above this plug. The UK and Norwegian requirements for this [79, 81] are that permeable intervals are isolated with primary seals placed above (and sometimes below) in impermeable rock.

Top and bottom seals used on oil wells generally involve milling at least a 30m (more often 50m) section of casing, then under-reaming to remove old cement and damaged rock. This procedure ensures removal of cement, settled mud or other debris from between the casing and the formation that could prevent the required multidirectional sealing. The milling and under-reaming that are used to prepare the volume to be occupied by the plug inevitably result in the barrier extending horizontally into some fresh rock as well as providing the vertical barrier up the hole. Hence the milled open-hole section has a diameter greater than that of the shallower hole sections that have not been reamed or through which casing remains.

After milling and under-reaming there is a wash-over to ensure a good cement bond and no contamination, then the cement or clay barrier is pumped to fill this window. To ensure there is no flow from the permeable interval during plug emplacement (which might contaminate the plug or lead to micro channelling) a mechanical or inflatable packer is usually placed immediately above the permeable interval, in an impermeable zone, and the seal is actually placed on top of this. These packers do not form part of the final seal, but merely isolate the permeable intervals from the primary seals as they are being placed.

Although under-reaming may expose or even remove fresh rock, using it in any attempt to remove rock damaged mechanically when the hole was initially drilled, or to re-establish a cylindrical geometry in a hole section that experienced breakout when drilled (see Section 4.3.6.1) is simply likely to lead to further breakout. This will occur as the stresses re-equilibrate to the new geometry (the same cylindrical geometry at which it failed initially), causing further shear failure and thereby potentially increasing the volume of damaged rock around the opening. Hence the under-reaming is only intended to remove the remnants of old cement and any rock that was damaged by the casing milling process.

Despite steel casing milling being widely used in PA for oil and gas wells, it is worth noting that there are some known drawbacks to this practice that might be relevant to any consideration of this approach for sealing GDF site investigation boreholes:

- a highly viscous drilling fluid must be used during the milling operation to lift the metal cuttings (i.e., swarf) to the surface;
- the swarf-laden fluids may have a density and viscosity that lead to the circulating pressure (or even just the static downhole pressures) exceeding, by some significant margin, the fracture pressures of the exposed formation (i.e., approximately equal to the minimum in situ stress in the rock). This high equivalent circulating density (ECD) can be sufficient to cause lost circulation and create artificial fractures in otherwise intact rock that may extend several metres from the well;

- in addition, it can be difficult to evaluate the effectiveness of the plug seals as subsequent pressure tests (via the tubulars remaining above the plug) cannot determine any differences between the quality of the cement seals in the casing annulus and the plug across the milled open-hole section. Also, such tests in an open-hole can only be performed up to the limit of the fracture pressure (approximately equal to the minimum in-situ principal stress) of the surrounding formation.

One oilfield solution to these problems, as an alternative to a milled window or just over sections where artificial fracturing might occur due to excessive ECDs, is a system known as perforate-wash-cement (PWC) [97]. This achieves remediation of any poor sealing by existing cement in the annulus, ensuring a good annular and lateral seal (over any desired length of hole) that can be tested and verified independently of the final plug inside the inner string. PWC also eliminates debris from milling, and hence the high ECDs associated with the removal of the swarf and risk of further damage to the rock surrounding the hole, but it does mean that sections of perforated casing remain down hole after PA.

Note that in the North Sea, and for most major international oil companies operating elsewhere, any casing left in the hole is always re-logged using sonic tools (see Sections 4.3.6.6 and 4.3.8) to identify existing channels and pathways in the annulus. If necessary it is perforated with shaped charges or abrasive jetting or milling tools, then the annulus is re-cemented in a similar technique to PWC. Despite steel casing not constituting a permanent barrier for PA, this re-evaluation of existing casings and cement is still performed. This is partly to ensure an improved PA beyond just the primary seals, but also to ensure the good annular seal needed for the verification (pressure) tests on the PA. See Section 4.3.8.

4.3.5 Plug emplacement

The downhole placement technique is critical to the success of any plug for PA of oil and gas wells. Other than when emplacing compressed clay-based pellets or nodules, the technique is to pump slurry.

4.3.5.1 Emplacement of cement plugs and clay-based slurries

Cement and powdered clays to be used as solid or liquid barriers in PA are generally pumped as slurries. Pressure requirements and pressure loss introduce limitations on physical properties, such as density and viscosity. Placement of slurries is achieved using through-tubing methods, including drill pipe, tremie pipes and coiled-tubing. After placement, cements are allowed time to hydrate and cure in order to create the required dense low-permeability solid barrier, before they are tagged (to determine their placement depth) and then tested/evaluated. See Section 4.3.8.

If weighted non-setting clay-based slurries are intended to remain as part of a PA, they are usually placed above and below cement plugs that provide barriers to prevent the slurry from mixing with any other fluids that might remain in deeper or shallower sections of the hole.

The normal emplacement process is the ‘balanced plug’ method, where the cement (or clay) slurry is pumped through tubing until the level of the material in the annulus is equal to that inside the tubing. The tubing is then pulled up slowly from the slurry and, in the case of cement, the mix is typically allowed 12-24 hours to harden.

Due to the risk of contamination from fluids already in the hole, larger volumes (than simply those needed to achieve the specified seal length) are usually pumped. For example, UK Oil & Gas [79] specifies at least 30m (100ft) of hydraulic seal is placed to provide isolation above each permeable interval. Worldwide, industry best practice is to set a plug of approximately 100 – 250m in length to ensure at least 30m of good plug is achieved, and in the UK 260m (800ft) or more theoretical seal height is always pumped; the actual amount varies according to the internal technical standards that the different operating companies have for PA of their wells.

Density control, mud removal, and slurry design are critical to effective cementing and plugging, especially to prevent gas migration. Hence, cement slurries are designed for suitable density, stability, setting times and rheological characteristics that will enable them to be pumped and conveyed to the required depths, and then emplaced without creating channels or potential fluid or gas migration pathways. Simulation and computer modelling are then performed prior to the actual well operations, to plan and optimize the cementing and plugging programme for the given slurry, borehole geometry, trajectory, and tubulars centralization etc. See, for example [98, 99, 100, 101]. Such planning helps to ensure that the cement is emplaced properly, displacing any fluids that were already in the hole so that channelling and potential fluid migration pathways are avoided when the cement hardens.

Special equipment and monitoring is then employed at surface to first ensure correct blending and mixing of the slurries, and to perform de-foaming that might result in air being entrained in the slurry. The cement mixing and pumping operations themselves can also be monitored, and further real-time simulations run, to further optimize the cement and plug placement [102, 103]. Once the cement has hardened a variety of methods are available to assess the seal quality. See Section 4.3.8.

Cement slurries are also frequently pumped in what are termed 'squeeze jobs', to inject cement into a formation or fractures for pressure- or fluid-isolation purposes. In a Bradenhead squeeze, the material to be squeezed is conveyed down a pipe or tubing, isolated from above using a top plug. Once on bottom, the entire casing/wellbore/tubing is pressurized from the top to force the material outwards from the borehole. In a packer squeeze, an expandable packer is run into the hole on the outside of a tubing, about 200-400ft above the zone to be squeezed. A volume of cement is pumped to bottom down the tubing, then the tubing and attached packer are pulled a short distance up the hole forcing the packer to expand and seal the annulus. The pipe is pressurized from above, forcing the cement in to the formation.

Some squeeze jobs involving clay-based slurries are also performed in the industry, but not those involving clay pellets as these solids cannot be effectively placed into the formation, into casing annuli, or behind casing through small openings such as perforations. Indeed, [74] prohibits the use of compacted bentonite as a squeeze material.

4.3.5.2 Emplacement of SANDABAND®

As explained in Section 4.3.3.3, SANDABAND® can be pumped via pipe or tubing as if it were a liquid, and it reverts to a solid when at rest downhole. If placed on a fluid it will sink, and therefore when it is conveyed downhole it is usually preceded by plastic granules that prevent it mixing with any displacement fluid already in the tubing or drillpipe. Similarly, after the SANDABAND® is pumped it is followed by plastic granules or similar to prevent it mixing with the displacement fluid that follows behind. Due to this risk of the SANDABAND® mixing with other well fluids at its top and base, larger volumes of this material (than simply those needed to achieve the specified seal length) are usually pumped.

4.3.5.3 Emplacement of clay pellets or nodules

Before emplacing compacted clay pellets or nodules, the wellbores are flushed and circulated with at least one hole-volume of water to ensure the removal of any material that might impede the swelling of the clays. In gravity placement, the compacted pellets or nodules are simply poured down the hole and allowed to sink. In a typical wash-down (or circulation) placement, the pellets or nodules are carried down a wash-pipe using a low velocity water flow. On leaving the bottom of the wash-pipe, the solids sediment downwards and the water returns up the annulus. Where such plugs need to be placed at some distance from the bottom of the hole they are simply placed above a gravel or cement bridge-plug. Typically water is maintained over the resulting plug for a minimum of 24 hours to ensure full hydration.

There is a recognised risk of such pellets/nodules bridging the borehole above their intended depth, due to them hydrating prematurely or because their placement and settlement is impeded by ledges and irregular sections of the borehole wall. The risk of them failing to reach the intended plug depth therefore increases significantly with both hole depth and hole inclination, to such a degree that the technique is only used in near-vertical wells and to depths of less than 4,000 ft. Indeed, there are prohibitions in the US [for example, 74] to their use in wells that deviate at more than 20° from vertical (i.e., dipping less than 70° from surface) or are deeper than 4000 ft. Where bentonite plugs do bridge above the intended interval they need to be removed (by drilling or using coiled tubing operations).

Note also that squeeze jobs are not conducted with clay pellets, and indeed their use in such situations are prohibited by some US authorities [74], as they cannot be effectively placed into the formation or into narrow casing annuli. However, cavity perforations are sometimes performed to allow Zonite to be placed behind large sections of casing.

Attempts have been made to seal old oil wells by dropping bentonite inside cardboard tubes [90], but this has only been done in cased shallow vertical holes and the method is certainly not a routine oilfield procedure. Otherwise, the conveyance of clay or other solid plug material inside pre-packed canisters or perforated tubing (run into hole using wireline, drillpipe or coiled-tubing) to form a plug is not currently used or proven in the oil and gas industry for PA of wells.

4.3.6 Hole quality and borehole damage

Breakouts and other borehole enlargements and damage are common occurrences in oil and gas wells. They impact drilling operations, logging and the quality of formation evaluation, casing and cementing, and result in abandonment in many rock types. With these problems costing the industry billions of dollars each year, considerable technology and knowledge has developed in the industry for predicting potential problems, adapting borehole designs and drilling practices to minimize their occurrence [104, 105, 106].

Achieving good hole quality across all or just selected formations means employing geomechanics data and analyses to help optimize well trajectories, select mud weights and mud types, choose casing points and hole sizes, and optimize drilling practices. Nevertheless, due to other constraints that dictate how wells must be designed and constructed and due to geological uncertainty, many wells still encounter enlargement problems and therefore boreholes need to be drilled with the knowledge that breakout and damage might occur. Other hole quality problems, such as key-seating and hole spiralling, can occur as a consequence of drilling practices and the characteristics of bottom hole assemblies (BHAs).

The technology and knowledge in the industry also extends to evaluating such problems when they do occur, and mitigating other operational problems that might follow [104, 105], including during PA. The same technology and practices would seem appropriate to the design and due diligence process for site investigation boreholes needed for a GDF.

4.3.6.1 Mechanical breakout

Mechanical breakout of borehole walls is most commonly associated with the rock undergoing shear failure due to excessive circumferential stresses that are induced around the opening when the rock is excavated. Where this occurs, and the damaged rock is removed from the borehole wall, classic wide breakouts develop and the hole can be enlarged over considerable depth intervals. See Figure 4-11.

Figure 4-11 Classic shear-induced wide breakout causing hole damage

In higher-strength and stiffer rocks that behave in an elastic-brittle manner, shear failure (when it occurs) tends to cause discrete fissuring, such that cavings fall into the hole (or can be encouraged to do so by swabbing the hole during tripping) to create well-pronounced breakouts. However, the damaged rock does not always separate from the borehole wall, and the result can be that the hole remains in-gauge but is surrounded by a BDZ that is broken and probably invaded by drilling mud. This is most characteristic of softer formations, where the behaviour and rock deformations may be more plastic, but it can still occur in many hard rocks. In either situation, wireline technologies, and some 'logging while drilling' (LWD) tools, are widely available to help identify and quantify such hole enlargement and residual BDZ. See Section 4.3.6.6.

4.3.6.2 Other shear and tensile damage

The focus on hole problems and near-well geomechanics in the oil and gas industry has led to an understanding of modes of stress-induced borehole damage [107]. Not all these modes of failure result in hole enlargement, and therefore a BDZ may still occur around an otherwise cylindrical hole. To assess and help prevent these different modes of damage, and to assess and correctly identify them when they do occur, geomechanics analyses is used in conjunction with the interpretation of borehole logs, borehole images and downhole pressure 'measurements taken while drilling' (MWD).

4.3.6.3 Other causes of hole problems

In addition to borehole damage due to stress-induced shear and tensile failures of the intact rock, there are other causes of borehole damage (Figure 4-12) that are more related to the nature of the formations, and to the drilling operation itself. Again, some of these can be prevented by geomechanics and drilling pre-planning to identify appropriate mitigation, and when they occur they can often be identified through wireline logs, borehole images and drilling measurements.

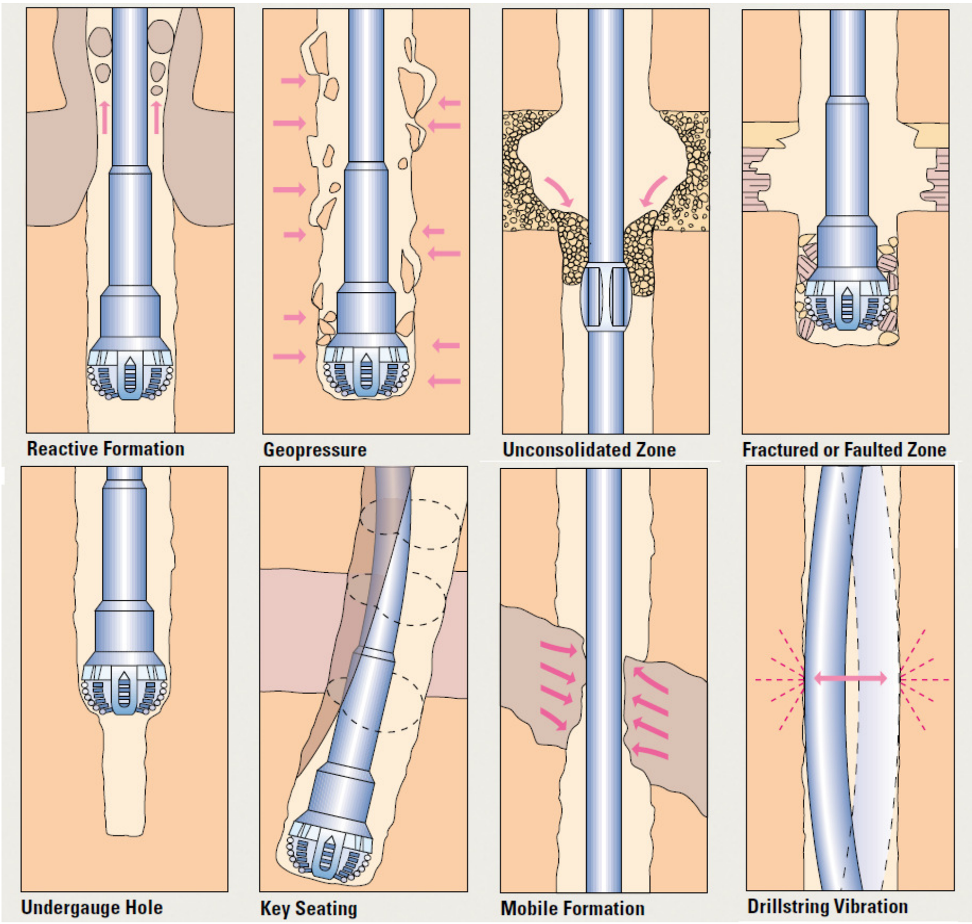


Figure 4-12 Other drilling-related and formation-related borehole damage [104]

4.3.6.4 Coring

Conventional coring in oil wells (i.e. coring to achieve maximum-diameter core rather than wireline-retrievable coring, which provides a smaller diameter core) is sometimes found to provide better hole quality than conventional drilling (i.e. using full-face bits, such as rock bits, PDC bits and diamond bits, and destructive drilling, rather than using core bits). There are a number of factors that might contribute to this, including:

- less aggressive tripping and drilling practices when a core barrel is in the hole compared to a conventional drilling assembly. This can lead to lower ECDs[1], less

[1] All other things being equal, the reduced annulus with a core barrel would increase ECD, but with lower flow rates (made possible with fewer cuttings being created by a core bit, hence less cuttings-loading in the mud-returns) and with less aggressive practices it can be possible to achieve lower ECDs than when routine drilling with a full-face bit. It is not given that this will always occur, and it has to be associated with the drillers focussing on achieving good core

surge and swap pressures, and less drillstring vibration that might otherwise contribute to poor hole conditions;

- the features of the core bits themselves, and less aggressive drilling that may be employed to ensure good quality sampling, can result in smoother borehole walls than achieved with other bit types and conventional drilling;
- the increased stiffness of a BHA for coring can help reduce or eliminate spiralling of the borehole that might otherwise occur with a less rigid BHA used for conventional drilling;
- the reduced annulus around the core barrel (compared to drill pipe) can help the barrel to smear the mud-cake at the borehole wall, helping to consolidate the borehole surface[1];
- coring operations can utilise special muds (over the cored sections) that are less aggressive and damaging to the rock than perhaps cheaper and more run-of the-mill muds used when drilling conventionally the other sections of the same hole;
- in some basement and other very competent rocks, having a reduced cross-section area of kerf (i.e., cutting face) from a core bit (compared to that of a full-face bit) can sometimes increase the rates of penetration. (For example, this has been proven in some of the quartzites and very hard shales in North African fields). In these situations, even allowing for the additional tripping needed to empty each filled core barrel, the time to excavate a long hole section can be significantly reduced below that needed with conventional drilling. Reducing the overall time spent in the hole, and the exposure of upper hole sections to a circulating fluid, can be beneficial to its condition.

However, conventional coring (as against reverse-circulation coring where small lengths of core are carried to surface by the mud, or wireline-retrieved coring) greatly increases the number of trips made in and out of the hole in order to empty the core barrel. This can increase the erosion and abrasion at one side of the borehole wall by the drillpipe and BHA, leading to significant borehole enlargement and key-seating (Figure 4-12) across build-up sections of inclined wells. The problem is exacerbated by the drill string forming a tangent that is pulled in to the inside curve of the borehole each time the core barrel is tripped out. Straight inclined hole sections can also be worn away to develop a similar key-seat and enlargement (whether coring or drilling) by the rotating drill string, which sits under gravity (even when under tension) against the lower side of the borehole. Vertical holes are not affected in these ways, but they can suffer key-seating due to drill pipes becoming locked against the borehole due to excessive mud weights and wall cakes (known as differential sticking).

In the case of different types of mechanical breakout and stress-induced damage to the borehole (as discussed earlier), the mechanisms causing problems are dependent on hole geometry (plus in situ stresses and pressures, overbalance between the mud weight/ECD

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rather than achieving maximum rates of penetration, but nevertheless it can help achieve better hole quality in cored wells.

[1] Some recent drilling projects (through 2012/13, in the USA) have utilised the smearing of a mud-cake against the borehole wall to help achieve improved stability and hole conditions. This smearing, achieved by the use of sections of larger diameter bottom-hole assemblies, and in some cases by the use of special shells that are deliberately designed to achieve greater contact with the borehole wall during rotation, has been found to provide a more robust mud-cake and improve overall hole quality. Work continues (in the UK and USA) to develop and better optimise muds specifically for this purpose. It is not a routine practice, and it definitely won’t always solve hole condition problems, but the technique has been found to be beneficial in some circumstances

and the formation pressures, well orientation, and the rock strength) rather than the way the hole geometry is achieved.

So whilst coring may improve hole quality, it needs to be emphasised that experience in the oil and gas industry is that, all other things being equal (i.e. annular velocities and hole pressures), it is not 'given' that hole quality will always be improved by coring. Indeed, when poor hole quality in oil and gas wells is a major risk, and because of additional risks to the overall operation that occur when coring, it is often abandoned in favour of conventional drilling to ensure that the well does reach the target depth without loss of hole or loss of equipment.

4.3.6.5 Reaming

Reaming a hole prior to running casing is normally unnecessary for oil and gas wells drilled to depth, regardless of whether the hole is drilled or cored, unless hole quality is poor, the drilling is through unstable or squeezing formations, or bit-wear has resulted in an under-gauge hole. Otherwise, bit sizes (both for conventional drilling and for coring) are simply selected to provide a hole of sufficient diameter for running and cementing the chosen casing string. Notwithstanding this, we recognise that 'wiper trips' are often necessary or prudent to ensure that the hole is clear; first before logging and then after logging but before running casing.

4.3.6.6 Borehole condition surveys

Mechanically- and chemically-induced wellbore instabilities are major causes for concern to the oil and gas industry, and result in billions of dollars of additional expenditure each year. Hence the industry has developed huge experience, technology and expertise (particularly in the subject of geomechanics) to help evaluate the potential for such problems in any formations drilled, designing and drilling wells through different rocks in ways that can help mitigate these problems, and assessing them when they do occur.

A selection of logging tools are used for the identification and quantification of hole quality, and/ or mechanical damage when it occurs.

- Multi-arm and acoustic callipers can reveal enlargement, and things such as borehole spiralling and rugosity, but not necessarily its cause and not the presence of damaged rock around an otherwise in-gauge hole. Hence calliper logs are, alone, not sufficient to understand the BDZ.
- Resistivity image logs (e.g., FMI wireline, and GVR LWD tools) can reveal the occurrence and mode of breakout, and even some damage that occurs without causing hole enlargement, but not the depth of alteration. Multiple passes of these tools can reveal the development of damage with time. See Figure 4-13 and Figure 4-14.
- Other resistivity (i.e. ARC LWD, and wireline high resolution laterolog resistivity array) tools can identify alteration and invasion (by mud) into natural and induced fractures, with multiple passes of these tools revealing how the damage progresses and evolves over time as the hole is drilled.
- Advanced sonic tools, employing a range of frequencies, can reveal the nature and extent of damage (both wall coverage and depth in to the formation).

Hence combinations of resistivity, sonic logs and calliper tools are normally employed in oil and gas wells to identify and assess the different aspects of mechanical damage to the borehole during drilling and with time. If casing is pulled or milled for a PA, the same tools can be run in the open hole to identify any borehole damage that might impact the successful plugging of the well.

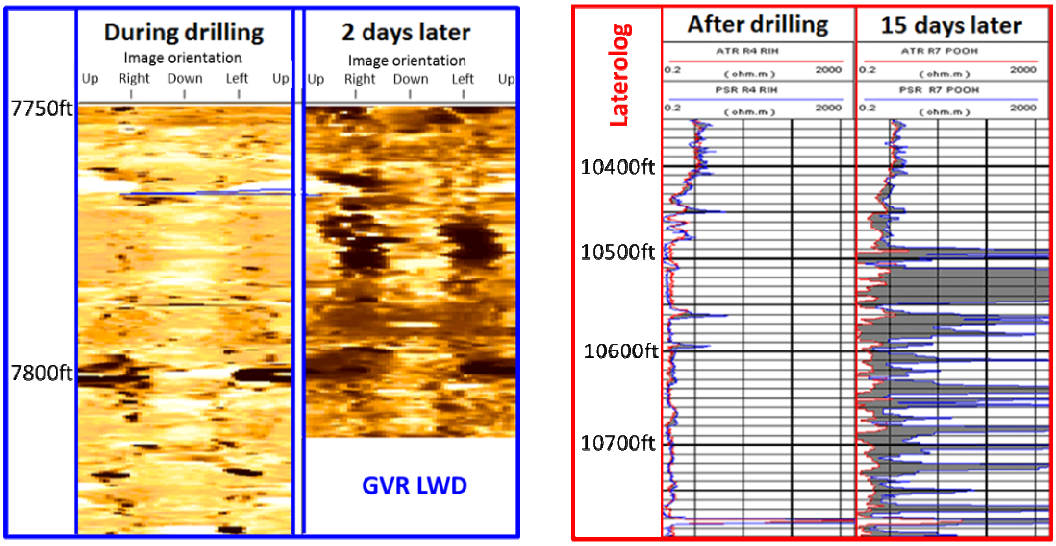

Figure 4-13 Evolution of BDZ and mud invasion into fractures identified from GVR LWD resistivity images and wireline laterolog resistivity

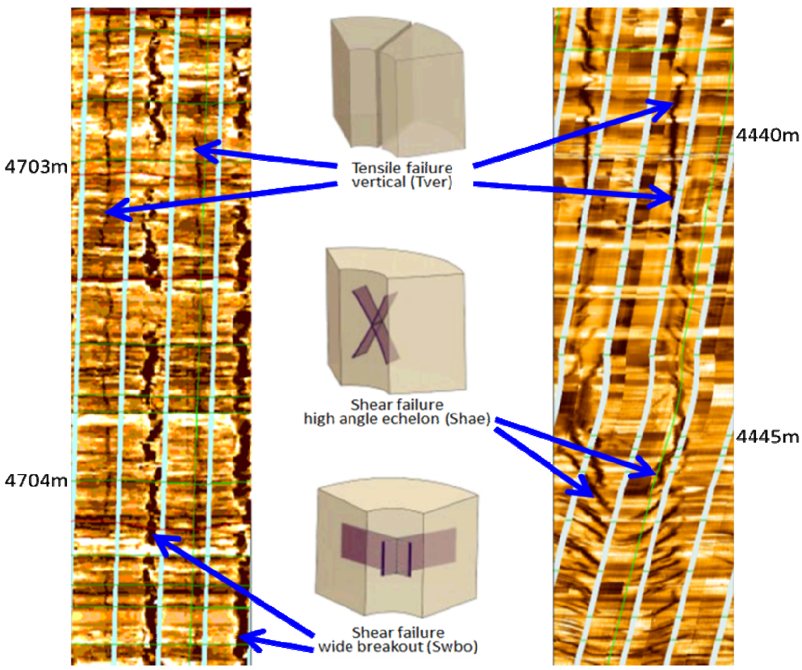

Figure 4-14 Borehole damage modes identified from FMI wireline resistivity image

4.3.7 Borehole design

With many oil and gas wells reaching the end of their useful lives, there is a realization now that many were designed and constructed without any consideration for their final PA, and that key to successful abandonment is the initial well design and well engineering. Hence wells planned and drilled now need to be designed also for their final PA [79]. For example, the choice of hole and casing sizes has a significant impact on the planning and complexity of any PA for oil and gas wells, Hence guidelines for PA [79, 81], and internal standards for major oil and gas companies, usually require PA to be taken into account in any initial design of a new well.

Nevertheless, as wells are designed and constructed individually (in terms of engineering, the formations and rock types they penetrate, and the drilling problems and hole conditions they encounter), they still need to be re-considered on an individual basis when the time comes for the actual PA.

In the oil and gas industry, wells having deviations in excess of 45 ° (i.e., dipping less than 45° from surface) are commonplace, and their drilling, logging, completion and PA are routine operations. Wells drilled to around 45° (deviation or dip) are handled (in terms of running casing, cementing, or PA) in much the same way as vertical wells, although we recognise that problems can occur with cuttings transport and hole cleaning. However, further complications do arise beyond around 50° deviation (i.e., less than 40° dip), due to density segregation in slurries (leading to development of channels in cement), saltation flow during circulation and pumping (rather than laminar or turbulent flow), and casing running. Also, as discussed in Section 4.3.5.3, complications can also occur when attempting to place plugs using compacted bentonite pellets inside wells inclined at more than 20° from vertical (i.e., dipping less than 70° from surface).

4.3.8 Assessing seal quality

A number of wireline tools are available to assess seal and cement quality in cased hole environments. Cement bond logs (CBL) [98, 108, 109] have been available for many years, and are used extensively across the industry. These pulse-echo sonic tools are conveyed downhole on wireline, and detect the bond of the cement to the casing and formation via resonance. Casing that is not bound has a higher resonant vibration than that which is bound, causing the imparted energy from the sonic signal to be transferred to the formation. Hence the amplitude of the waveform of the resonance is the basic measurement that is evaluated for potential micro-annuli that may provide a pathway for liquid or gas migration.

Variants of CBL, combined with neutron density measurements that can be run in a single pass, are also available (including for slim-holes where casings are less than approximately 7” outer diameter, and for conveyance using coiled-tubing). These provide more detailed information on cement quality and integrity, and for PA applications can be used to identify sections of casing to be left in the hole that might require perforating and remedial cementing. See Figure 4-15.

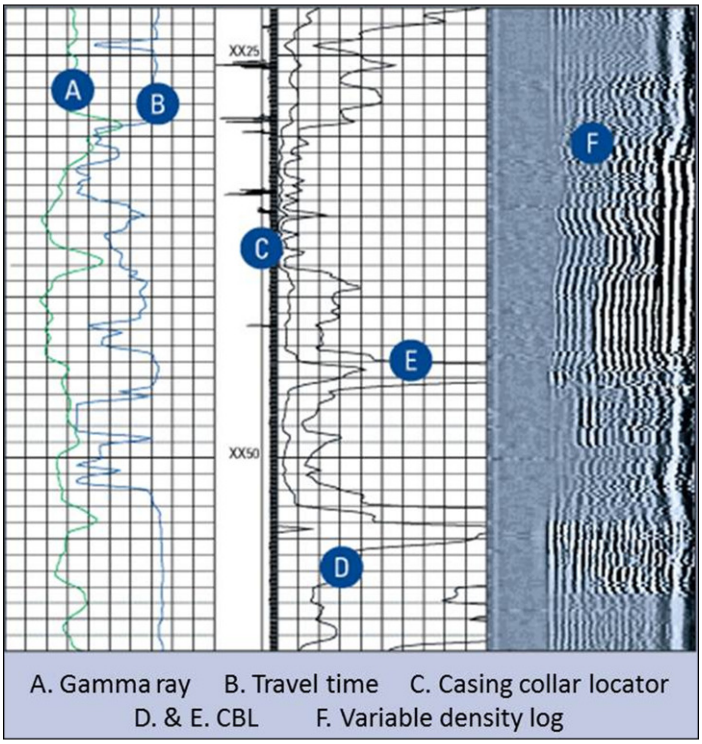

Figure 4-15 CBL and density log data to identify quality of cement behind casing

Ultrasonic imaging tools [108] that combine azimuthal measurements of signal attenuation with those of resonance are a more recent development and allow the identification of any channels in the cement. More advanced versions of this technology [110], employing also flexural waves, are able to detect low density solids behind the casing from liquids. Moreover, their azimuthal coverage allows imaging around the entire circumference of the casing, with a solids-liquid-gas map pinpointing any channels in the cement and confirming the effectiveness of zonal isolation. Third-interface echoes (TIEs) provide additional information on the position of the casing within the borehole, the borehole shape, and any casing corrosion that may have already occurred. Such tools are thus able to provide a more complete understanding of the seal quality than just CBL and density measurements. See Figure 4-16.

The quality of the cement bond and seal behind any casing that is to be left in the hole is of paramount importance to the success of a PA. Hence, in the oil and gas industry, casing left in the hole is always re-logged to identify channels and pathways in the annulus. If a poor cement seal is found to exist, these logs can be used to determine the most appropriate solutions and procedures (such as perforating, cement squeeze, plug setting, pipe cutting, section milling etc.) to correct the problem.

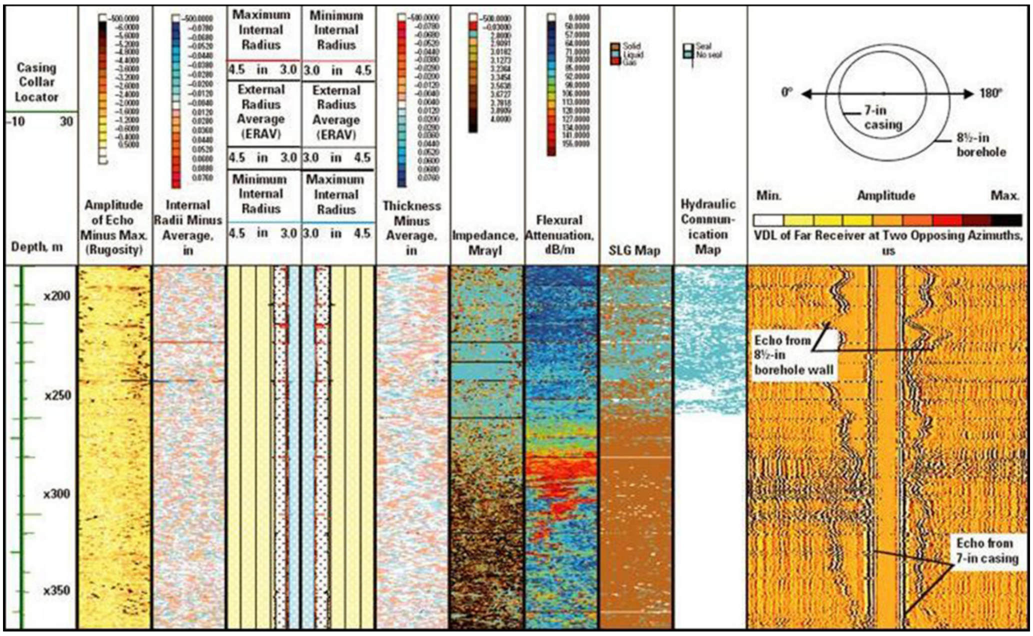

Figure 4-16 Isolation Scanner results showing formation, casing, cement and micro-annulus data

Cased-hole logging, to measure formation and fluid properties behind casings, is also widely employed throughout the industry. This employs techniques other than the acoustics and ultrasonics used for cement logging, such as resistivity and pulsed neutron. Advanced sonic tools, employing a range of frequencies, can also be used to see behind casing to provide information on the formations, such as their mechanical properties.

Having used logging to establish the likelihood of a good seal, pressure tests are performed on each casing annulus to verify isolation. Likewise, the effectiveness of cement plugs are also assessed through pressure testing. We note that there are currently no logging tools or technologies available to the industry that might provide any look-ahead capability to 'see' into the plug using acoustic, resistivity or density techniques.

Positive pressure tests are performed by pressurizing the wellbore from above, utilizing mechanical or inflatable packers to isolate any upper sections of the hole that are not to be evaluated at this stage. These are liquid pressure tests on a shut-in well, in which an additional well-head pressure is applied to the borehole fluids inside the hole. After pressurizing the borehole section to the desired amount, the system (sealed at top, with pressure measurement devices installed) is monitored to record any decay in pressure that would indicate a leak downhole. The degree and duration of pressuring depend on the requirements that have been specified for each seal, but usually a minimum of 500 psi (approximately 3.5 MPa) above the surrounding formation pressure is the target pressure for a positive pressure test.

Negative pressure tests (i.e., inflow tests) are performed by drawing down the pressure in the wellbore to below the formation pressure at depth, by introducing a lower-density fluid column or evacuating fluid from the wellbore, then monitoring for any pressure increase in the sealed system due to influx from the formation outside. Where the formations themselves contain gas, there could potentially be ingress of gas into the well, which would be detected as an increase in pressure inside the well.

Where the top of the cement is inside a casing above the milled window, a pressure test will only assess the quality of the seal provided by the cement inside the casing. It will make no determination of quality of cement in the casing annulus or in the milled open hole. Similarly, a pressure test on a plug with its top in a milled or other open-hole section cannot determine any differences between the quality of the cement seals in the casing annulus and the plug across the milled open-hole section. One solution to this is to validate the seal in the annulus by using a +ve and/or –ve pressure test in the hole after a perforate-wash-cement (PWC) treatment has been performed (see Section 4.3.4).

Other tests that are performed to verify emplaced plugs (prior to them being pressure-tested) are:

- the position of the top of the barrier is verified by tagging (using a tubing string or drillpipe) or by measuring (i.e., wireline, calibrated for stretch and temperature effects);
- in the case of hardened cement plugs, weight tests. These are normally performed using the mass of the drillpipe, with loads being estimated from the hook-load at the rig and an estimate of the buoyancy provided by any fluid in the hole. With this technique loads of approximately 10,000 to 15,000 lbs (for typical UK oil and gas wells) are applied. Load tests using the weight of wireline- or tubing-conveyed equipment are limited by the tools in the hole and the hole inclination.

With such a wide range of conditions and PA scenarios being encountered in the oil and gas industry, requirements for assessing seal quality and verifying sealing and pressure isolation vary tremendously. Guidance on the verification requirements for UK oil and gas wells are provided by [79] and summarized below in Table 4-3.

Barrier type		Verify barrier position/length	Assess seal
Cased hole	Annulus	Verify good cement along >100ft interval if logging or test over 1000ft interval above plug if estimated	+ve pressure test or -ve pressure (inflow) test
	Plug	Tag or measure	Weight test then +ve pressure test
Cased hole set on plug/barrier	Annulus	Verify good cement along >100ft interval if logging or test over 1000ft interval above plug if estimated	+ve pressure test or -ve pressure (inflow) test
	Plug	Tag or measure	Weight test then +ve pressure test
Plug set in open hole	Plug	Tag or measure	Weight test

Table 4-3 Summary of guidance on plug and seal verification for PA of UK oil and gas wells [79]

4.3.9 Other considerations

4.3.9.1 Thermal environment

Temperatures encountered by oil and gas wells drilled to reservoir depths are routinely in excess of 55℃, frequently in excess of 100℃ , and in the case of high pressure high temperature (HPHT) reservoirs and environments in excess of 150℃. In the UK [79] a number of issues specific to HPHT wells are taken in to account in relation to these well design and PA (i.e., temperature cycling, high depletion and potential recharge, and cement degradation). For Norway [81], there is additional emphasis on the stability of any fluids left in the hole forming part of the PA. But neither set of guidelines have special requirements relating to lower temperatures (say to only 55℃ or even 100℃).

4.3.9.2 Permafrost

In the oil and gas industry, potential natural changes (caused by natural evolution of the geosphere) that might impact the longevity and effectiveness of a PA are not generally considered. For Alaska, where oil wells are routinely drilled through permafrost and where melted permafrost may re-freeze around wells after their PA, there is only minimal guidance [72] in that any cements must be designed to set before freezing occurs, and that they should have a low heat of hydration. There are also requirements for any well fluids left in the hole between plugs (as part of the PA) to have freezing points below the temperature of the permafrost and to include corrosion inhibition so they do not degrade any steel casings that have been left in place. Guidance from the regulators in Canada is similar.

4.3.9.3 Seismicity

Seismicity is a consideration for the oil industry with regard to induced and natural seismicity affecting well survivability and environmental impact of oilfield operations, but it does not feature in PA planning. It may be that short sections of wells passing through mobilized faults (which might be the source of the seismicity) could be sheared locally. This is certainly what is experienced in oil and gas fields where there is tectonic activity, but such a localised mechanism would be unlikely to affect the overall performance of the total sealing system for a wells PA. A greater potential for fluid movement between formations probably comes from the mobilized faults themselves, if they were to become more conductive to fluids by dilation or other alteration. Again, such effects are seen in and above some oil and gas fields that are deformed due to depletion or subjected to seismic events.

4.3.9.4 Perturbation of rock stresses or groundwater

The return to normal conditions after the completion of a major project will lead to stress re-distributions in the surrounding rock that might impact nearby boreholes that have already been sealed and abandoned. For example, drainage/injection and associated pressure changes that occur with oil, gas and water extraction can causes stress alterations and rock deformations across entire fields and aquifers, leading to well integrity problems [111] and even impacting adjacent fields and formations.

Hence potential changes to groundwater pressures and flow patterns is a consideration for the PA of oil and gas wells; not with regard to natural changes that might occur but rather with regard to wells located in parts of an oilfield that may subsequently experience water flooding or water injection to aid hydrocarbon recovery. In the UK [79] any PA must consider future fluid movements through permeable formations that might potentially occur in the future in association with operation of the field.

4.4 Experience from CO_2 storage

4.4.1 Introduction to CO_2 storage experience

The storage of CO_2 in deep geological reservoirs is being actively researched throughout the world as a possible means of reducing anthropogenic CO_2 emissions to the Earth's atmosphere and thereby helping to prevent unacceptable anthropogenic climate change [112, 113, 114]). This option involves capturing CO_2 at fossil fuel power stations or other large point sources, such as steel works or cement works, compressing the CO_2 to form a supercritical fluid and then pumping it into an underground geological reservoir. Most reservoirs being considered fall into two main categories:

- depleted hydrocarbon reservoirs;
- so-called "saline aquifers", which are porous and relatively permeable rock formations filled with saline water or brine.

At the time of writing, the technology has not been fully deployed on a full-cycle, commercial scale, involving CO_2 capture, pumping to the reservoir and underground storage. However, there have been a number of pilot-scale and large-scale demonstration projects during the previous 18 years or so. The first large-scale demonstration was the offshore Sleipner project, which commenced in 1996 in the Norwegian sector of the North Sea [115]. Globally there were 12 projects in operation in February 2014 while a further nine were being constructed and another 39 were in various stages of development planning, of which six may make a final investment decision during 2014 [114].

CO_2 injection for enhanced oil recovery (EOR, rather than CO_2 injection for storage or disposal) is more widespread and established, often involving reinjection of CO_2 recovered to surface during oil and gas production from other wells and fields. The first instance of CO_2 EOR was in Texas in 1972, and the largest CO_2 EOR project to date is the Weyburn field in Canada, which has been in operation since 2000.

4.4.2 Experience of sealing

To date CO_2 storage projects have employed standard well sealing practices that have been developed by the hydrocarbons industry and typically use the following major components (see Figure 4-17, after [112]):

- a steel casing (which may be removed in some applications);
- a cement grout used to fill the gap between the steel casing and the surrounding rock; and
- a cement plug sealing inside the well.

A cement sealing plug will provide the main barrier to CO_2 migration through the well. However, it is recognized that care is needed to use cement that is sufficiently resistant to degradation owing to the action of CO_2 [112]. Cements that are resistant to CO_2 have been developed for oil field and geothermal applications, notably for EOR using CO_2 (e.g. [116]).

There have been some concerns that any casing left in the borehole might corrode in the presence of CO_2-charged water and thereby create pathways for CO_2 migration [112]. A suggested solution to this potential problem is to remove the casing and the liner, where it penetrates the caprock to the storage reservoir. In this case a cement plug can be put into the open borehole (Figure 4-17, right).

The seal quality between the cement plug or casing-cement bond and the penetrated caprock is recognized to be a potential concern [112]. Drilling or milling operations could cause microchannels to develop near to the wellbore. To prevent these channels from forming pathways for CO_2 migration, they must be sealed with cement. A further strategy for improving the quality of the cementing is to flush the storage reservoir, thereby displacing the CO_2 from the environs of the well bore so that it cannot interact with the cement while the cement cures.

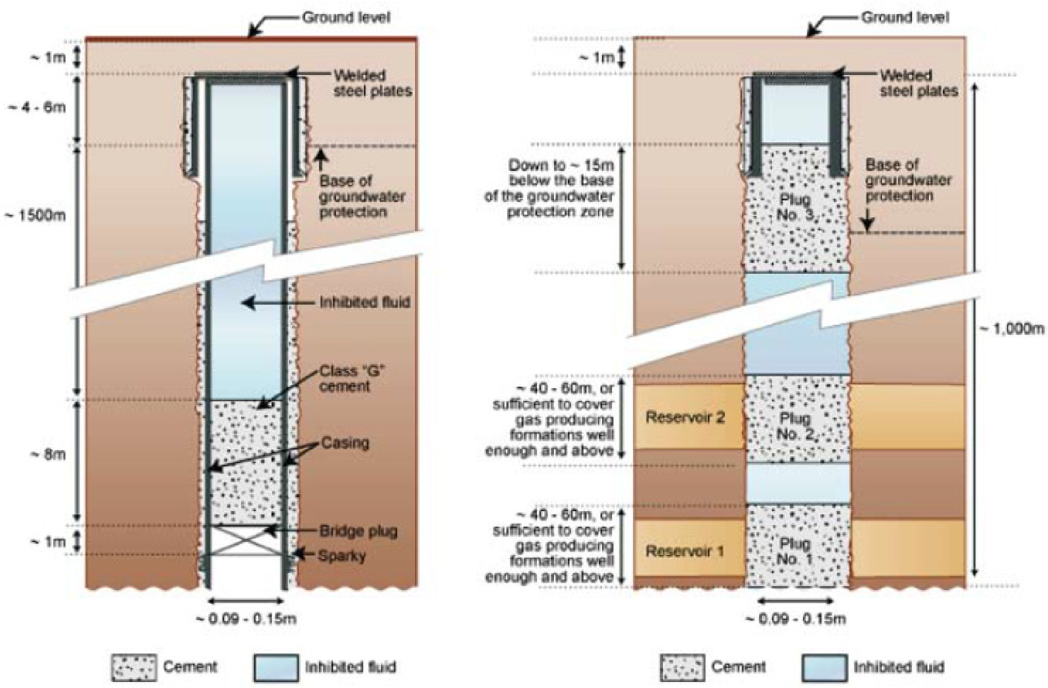

Figure 4-17: Examples of how cased (left) and uncased wells (right) wells are abandoned (after [112]).

There has also been research into borehole sealing in salt by Clausthal University of Technology at a gas field in Altmark where Enhanced Gas Recovery (EGR) using CO_2 was tested ([117], [118]). The aim was to develop borehole sealing, using natural materials, for long-term sealing of boreholes in CO_2 storage sites. It has been investigated whether open boreholes might be adequately sealed by encouraging the salt (halite) cap rock to creep inwards and seal the open-hole. This would be achieved by reducing the mud weight in the hole, thus reducing the mechanical support to the borehole wall and thereby helping to accelerate the rate and magnitude of creep deformation back in to the hole. If this proves feasible, it could deliver a PA where the caprock truly is restored to its original state. For the remaining clay/marl/shale overburden at the Altmark site, bentonite would be placed in the open hole to try and recreate the natural barrier.

4.5 Experience from water resources industry

4.5.1 UK experience

In the UK, the Environment Agency (EA) is the regulator responsible for protecting groundwater resources. EA has recently issued updated good practice [13] on decommissioning redundant boreholes. More detailed information is presented in [119].

With regard to water resource protection, EA guidance [12] identifies overall objectives for seals and backfill:

- removing the hazard of an open hole (safety issues);
- preventing the borehole acting as a conduit for contamination of groundwater;
- preventing the mixing of contaminated and uncontaminated groundwater from different aquifers;
- preventing the flow of groundwater from one geological horizon to another;
- preventing the wastage of groundwater from the overflow of artesian boreholes.

A number of potential approaches are presented in EA guidance, and are discussed further below. With regard to permeability, the requirement is either to mimic the permeability of the surrounding rocks and soils or to place a low permeability backfill throughout the borehole.

Longevity of seals and backfill is not discussed in [12]. Removal of casing is only to be considered '*where the casing has corroded or broken, or the grouting has failed*'. Cement, grout or concrete are shown as seal or low permeability backfill materials in the guidance. The implication is that sealing is required on timescales of order hundreds of years.

The EA guidance [12] defines five steps for decommissioning redundant boreholes, which are summarised below. Text taken directly from the guidance is given in italics.

> *Step 1: defining the objectives*. The method of decommissioning the borehole should address the five objectives listed above;
>
> *Step 2: removing headworks and casing*. Any pumps, piping and infrastructure in the borehole must be removed before sealing. The circumstances when casing is to be removed are described above;
>
> *Step 3: backfilling*. The good practice document states '*For most purposes the ground should be restored as closely as possible to its pre-drilled condition*'. Alternatively, the entire borehole can be backfilled with low permeability materials. Schematic options for decommissioning boreholes are shown in Figure 4-18. *Cement, grout or concrete* are shown as seal or low permeability backfill materials;
>
> *Step 4: sealing the top of the borehole*. The backfilled borehole should be completed with an impermeable plug and cap. The top 2m should be filled with cement, concrete or bentonite grout;
>
> *Step 5: recording details and informing others*. Accurate records should be kept, and EA and British Geological Survey notified.

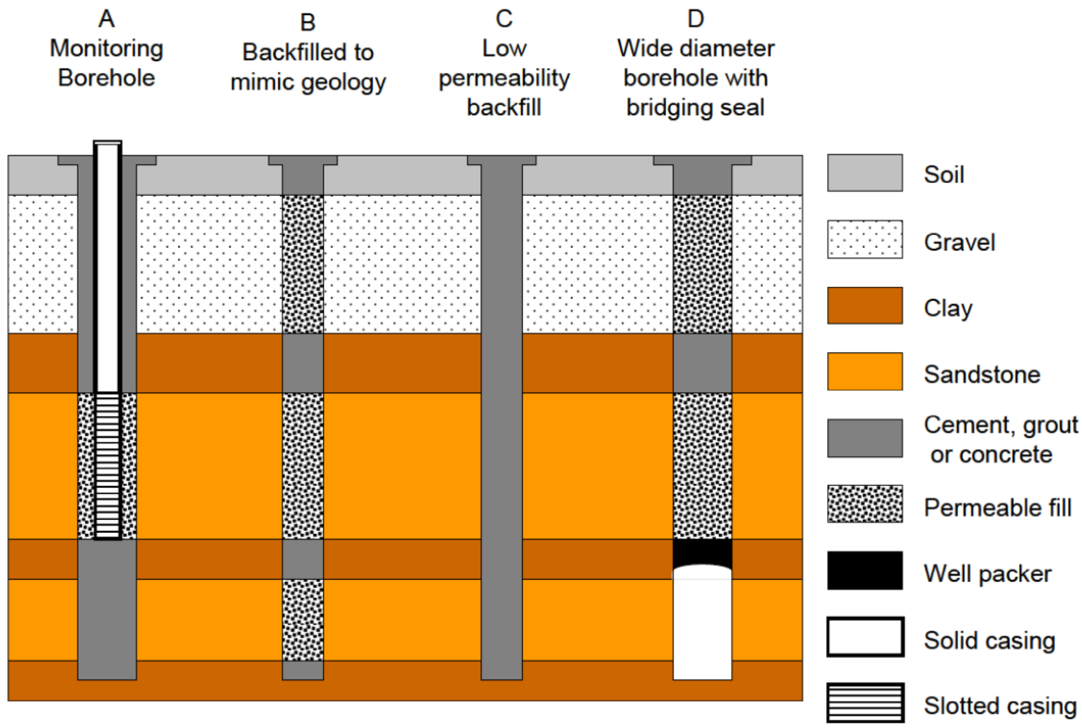

Figure 4-18 Schematic options (B-D) for decommissioning boreholes. From [13]

Cement-based materials and bentonite are both commonly used to seal boreholes for groundwater resource protection. The material is generally pumped into place as a grout through tremie pipes. In the case of cement, bentonite is commonly added, generally up to 5% by weight. Bentonite is added to cement for two principal reasons.

- Firstly, to improve the properties of the grout during placement; addition of bentonite provides for a longer pumpability at normal pressures as a result of delaying strength development. It also increases slurry viscosity and consequently reduces fluid loss to the formation.
- Second, the addition of bentonite improves the sealing properties of the cement. The aim is for the seal/plug material to have mechanical properties similar to those of the surrounding rock, so that seal and rock deform in similar ways. This reduces the potential for cracks to open at the interface with the rock. Addition of bentonite reduces the strength of the product; bentonite proportion is adjusted to suit the rock type. Also, addition of bentonite reduces the potential for shrinkage and cracking, so providing a better seal in the borehole.

An alternative approach, generally used for shallower boreholes, is to seal using bentonite pellets. The bentonite pellets are generally placed through tremie pipes, to reduce the possibility of them bridging in the borehole.

The most relevant UK example of backfilling boreholes for groundwater resource protection is provided by the Nirex site investigation for a GDF near Sellafield. Backfilling of site investigation boreholes is described in detail in [10]. In summary, the fully cemented steel casings were regarded as a permanent system that would provide the required protection for the freshwater aquifer. They were therefore left in place. Where required (because of the potential for contamination of the freshwater aquifer by saline water at depth), open sections of borehole were sealed using a plug of cement/bentonite grout. A series of trials with different cement/bentonite formulations was undertaken to determine the suitability of mixtures in terms of pumpability, segregation, density and compressive strength characteristics. The addition of bentonite *resulted 'in a low-shrink, low permeability grout which was considered would produce the required high quality seals'* [10]. The target mix adopted for most boreholes was: 950 kg water; 520 kg OPC; 250 kg bentonite powder. The grout was prepared using industry-standard equipment and emplaced by pumping.

The proposed approach to sealing these boreholes was accepted by EA.

4.5.2 US experience

In the US, the Standard Guide for decommissioning of groundwater wells, vadose zone monitoring devices, boreholes and other devices for environmental activities was re-approved in 2012 [120]. The objectives are broadly as in the EA good practice guide; to ensure the physical structure of the well does not provide a means of hydraulic communication between aquifers or react chemically in a detrimental way with the environment. As the guide is intended for use on sites where solid or hazardous materials or wastes are found, sealing is stated to be required '*over the period of time that hazardous materials are found at the site'*; this suggests typical timescales of tens to hundreds of years.

Ideally, casing should be removed by pulling or over-drilling. If this is not practicable, it is stated that sections of plain casing can be left in place provided that the *'grout in the annular space can be verified to be in good condition'*. Typical practice, after preparing the borehole to ensure it is free of debris and foreign matter that may restrict the adhesion of the plugging materials to the borehole wall, is to pump the plugging material to the base of the borehole using a tremie pipe. A wide range of *'plugging materials'*[1] is identified as potentially suitable, depending on ground conditions. See Table 1 of [120], where the full list of materials is given. The materials include:

- a range of OPC-based cements. Variants with moderate and low heats of hydration, high early strength and high sulphate resistance (relative to the most commonly used type) are listed. Another variant (Type K) is defined as *'expansive cement'* and contains additions such as tricalcium aluminosulphate to provide for expansion;
- pozzolanic cements;
- bentonite, as pellets, chips, granules, powder and slurry.

A number of materials are added to cement to modify its properties. The most commonly used additive is bentonite; OPC – bentonite mixtures are commonly used to seal boreholes for water resource protection. Bentonite is added, generally up to 4% by weight, for the two principal reasons outlined in Section 4.5.1: improvement of properties

[1] Plugging materials should be carefully chosen for well closure to be permanent. Required characteristics of plugging materials include:

- should not adversely react with groundwater or geological materials;
- should have hydraulic conductivity that is comparable to or lower than that of the lowest hydraulic conductivity of the geological material being sealed;
- must maintain sealing capabilities over the required time and not degrade due to chemical interaction, corrosion, dehydration, or other physical or chemical processes;
- should not be readily susceptible to cracking or shrinkage, or both;
- must be capable of forming a tight bond and seal with well casing and the formation.

during placement and improvement of seal properties. OPC types are stated in [120] to form good seals in boreholes when used with bentonite in 3 to 5 % concentration.

4.6 Discussion

Chapter 4 presented the approach to abandoning/decommissioning boreholes taken by a number of organisations and industries: RWMOs, oil and gas industry; CO_2 storage industry and water resource industry. This section summarises this experience, some of which is highly relevant to RWMD's future RDD programme for borehole sealing. Implications for RWMD's programme are not discussed in this section. Instead the key issues, which are informed by this section, the companion section on the evolution of seal properties after placement (Section 5.6) and the results of illustrative calculations (Chapter 6) are discussed in Chapter 8.

As a general point, we note that borehole diameters and depths of potential relevance to RWMD (from 6¼ " to 36" diameter and to depths to 2000m) are fairly typical of onshore and shallower offshore oil and gas wells. Likewise, oil and gas drilling encounters many rock types worldwide, from weak overburden, through competent sedimentary formations, to hard basement reservoirs. As such, there is considerable technology and knowledge in the oil and gas industry on borehole sealing that may be appropriate to deep site investigation boreholes for GDF.

4.6.1 Approach to abandoning/decommissioning boreholes

The approach to abandoning/decommissioning boreholes is broadly consistent across the industries considered, although this is sometimes obscured by the different nomenclatures used. The main common themes are:

- sections of boreholes are sealed to prevent or reduce to an acceptable degree the movement of fluids through the borehole for as long as is required. Seals must have sufficiently low permeability and sufficient longevity to meet these requirements;
- the intervals between the seals are filled with materials (described as 'plugs', 'backfill' etc.) that provide mechanical stability for the surrounding rock and overlying and underlying seals. Additionally, these materials greatly reduce the permeability of the section relative to that of the open borehole, although this is not their primary function. Lengths of cemented casing often remain in-situ between the seals; in this case, the cemented annulus rather than the material filling the casing provides the resistance to flow through the section;
- seals (or 'key zones', 'primary seals' etc.) are placed across lower permeability sections of rock in uncased sections of hole. Their lengths depend on the rock properties and sealing concept; 30m or more is typical. Working in conjunction with the surrounding rock, they restrict fluid movement along the borehole. Seals are not placed directly across high permeability horizons.

4.6.2 Selection of materials for seals

The required longevity of a borehole seal has a strong influence on material selection. For RWMOs, post-closure borehole seals must function on timescales required by post-closure performance assessments. These timescales depends on the repository concept and the regulatory regime. For example, SKB requires a 100,000 year lifetime from its post-closure clay seal, which is designed to seal key horizons in the repository host rock.

The oil and gas industry considers that sealing is required on the scale of ~1,000 years, beyond which borehole collapse and the associated natural movements of the formation surrounding the PA are considered sufficient to maintain the seal to the reservoir. In order to mitigate climate change, the CO_2 storage industry requires that borehole seals must be effective for at least several thousands of years. Finally, the water resources industry is not explicit about timescales, but the guidance suggests required timescales of hundreds of years (i.e. commensurate with the lifetime of cemented casings).

Because of the very long timescales involved, RWMOs generally select natural materials for post-closure seals. Bentonites or bentonite-based materials are proposed for use in both HSR and LSSR, though barite has also been proposed as a seal for the latter. In evaporite rocks, seals formed from both salt-saturated cements and natural evaporite minerals have been used or proposed. Note that long-term creep of evaporite rocks around a borehole is expected to contribute to sealing.

Portland cement seals are most commonly used in the UK oil and gas industry although, in the US and elsewhere, more than a thousand wells (typically vertical and less than 1,000m deep) have been successfully sealed using bentonite pellets. For deeper and deviated boreholes, the emerging solution in the oil and gas industry is SANDABAND®, a pumpable mixture of bentonite and barite plus up to 75% quartz sand. For CO_2 storage, cement seal concepts currently provide the main barrier to CO_2 migration through the well. Research into the use of natural evaporite seals created by long-term creep of rock around the borehole is also in progress. Portland cement or mixtures of cement with other materials (commonly bentonite, up to 5% by weight) are widely used to seal boreholes for water resource protection. It appears that cement-based sealing solutions are widely used when the required lifetimes are of order a thousand years or less.

4.6.3 Selection of materials for intervals between seals

Portland cement or mixtures of cement with other materials are commonly used to fill intervals between seals. In the SKB concept for HSR, higher permeability zones between clay seals are filled with 'concrete plugs' (a mixture of 4% low-pH cement[1] in quartz sand). The Nagra concept for LSSR involves placing expanding cement in the intermediate zones. In the oil and gas industry, materials used to form seals (typically Portland cement; sometimes bentonite) are also used to fill cased sections of borehole. Two approaches are commonly used for water resources protection. Firstly, either low-permeability cement-based seals or bentonite seals are used throughout the borehole. Second, higher permeability sections are backfilled with (unspecified) materials that mimic the permeability of the surrounding formation; cement-based or bentonite seals are used to seal lower permeability horizons.

4.6.4 Removal of casing

The required lifetime of the seal also influences the approach to cemented casings. IAEA guidance for sealing boreholes at sites for geological waste disposal is that casing be removed prior to sealing. This will not be possible in some situations (refer to Section 2.2.3); in these circumstances, it is recommended that casing be locally removed to enable local seals to be placed in contact with the rock. The oil and gas industry also recognises that cemented steel casing does not constitute an everlasting barrier to lateral flow into or out of the well. However, in most oil and gas PAs, at least some steel casing will be left in the hole simply due to the huge costs and logistics needed to remove it. A

1 See Section 3.7 of [57] for further information on low-pH cement

similar approach is adopted for CO_2 storage. To ensure longer-term sealing is achieved, a frequent requirement is that casing is locally removed in at least one location and a seal placed in direct contact with the rock. At the other end of the spectrum, for water resource protection, cemented casing is left in place to form part of the sealing system provided that it is in good condition.

4.6.5 Placement of materials

Across the industries considered, materials are generally emplaced into boreholes as 'suspensions', 'grouts' or 'slurries' using tremie pipes or equivalent. This is always the case with cements and cement-based materials (e.g. cement-bentonite mixtures) and with sealing materials formed from evaporite minerals. Bentonite-based materials are also sometimes emplaced in this way. For example, SANDABAND® is emplaced in oil and gas wells by pumping.

Bentonite and bentonite-based materials can also be emplaced as pellets and as pre-formed blocks. Bentonite pellets (without mineral additives) are widely used in the US to seal oil wells up to 1,000m deep. Pellets are also used as the emplacement method for some RWMO applications; for example, Quellon-HD® is a bentonite – magnetite mixture used as the seal material in the Nagra borehole sealing concept. The only example of emplacing bentonite as pre-formed blocks is provided by the SKB clay seal concept.

Overcoring of sealed borehole OL-KR24 at Olkiluoto demonstrated that the bentonite seal was placed at the correct depth in the borehole using the SKB Basic Concept. In contrast, the concrete plug, which was emplaced by pumping, was offset by 5m from its correct position. This demonstrates the potential uncertainties associated with pumping materials into place and is one of the advantages of controlled emplacement through a container, as in the SKB Basic Concept. Whilst the problem in OL-KR24 may relate to the pumpability of the material (it may have hardening too quickly) and therefore could be overcome by further development work, the oil and gas industry also recognises uncertainties in accurately predicting the upper level of materials pumped into boreholes, mainly due to unexpected losses from the borehole into permeable zones.

In the oil and gas industry, cement slurries are frequently pumped in what are termed 'squeeze jobs', to inject cement into a formation or fractures for pressure- or fluid-isolation purposes. Some squeeze jobs involving clay-based slurries are also performed in the oil and gas industry. These approaches have the potential to partially seal the BDZ. Note that bentonite pellets are not used in the oil and gas industry for squeeze jobs, because these solids cannot be effectively placed into the formation, into casing annuli, or behind casing through small openings such as perforations. Some RWMOs consider whether bentonite placed as solids in large openings such as tunnels could expand into the disturbed zone and partially reverse it. However, application of this in a borehole environment does not seem feasible and would be very difficult to prove that it works successfully.

4.6.6 Single materials or mixtures?

In the industries we have reviewed, some seals have been formed from single materials: for example, bentonite seals and cement seals. Other sealing materials are formed from mixtures: for example, cement-bentonite, bentonite-magnetite (Quellon-HD®) and quartz-barite-bentonite (SANDABAND®). Mixtures are used:

- when they improve placement properties, such as increasing the density of bentonite pellets or increasing the pumpability of a cement. This has the additional effect of reducing costs, through reducing effort and rig time;
- when it is considered they improve sealing performance, such as reducing shrinkage and strength in cements or though reducing bentonite erosion by addition of an inert sand fraction.

Recent experience in the oil and gas industry is that there is a move away from mixtures such as small proportions of bentonite in cement because they can compromise the way the individual sealing materials work. They also have the potential for density segregation and particle aggregation during placement, which could lead to the formation of a heterogeneous barrier. Interestingly, cement – bentonite mixtures are still used extensively for sealing boreholes for groundwater resource protection.

A final concern about mixtures arises if the different components are not chemically compatible. Whilst interactions are not expected to result in significant changes to seal properties over engineering timescales, longer-term sealing performance might be compromised. This is considered further in Chapter 5.

5 Evolution of seal properties after emplacement

5.1 Introduction

This Chapter presents information on the evolution of seal properties after placement of the seal. The information is taken predominantly from outside the RWMD programme. We review the approaches taken in a number of radioactive waste management programmes and in other industries (oil and gas; CO_2 storage; water resources) to build understanding of seal evolution. We present the key issues identified by these programmes. This chapter will make clear that the selection of materials for borehole seals is strongly influenced by the required lifetime of the seal.

5.2 Experience from radioactive waste management organisations

5.2.1 Introduction

There is extensive accumulated experience regarding the long-term behaviour of sealing and backfilling materials, mostly assessed from a viewpoint of using the materials at the scale of an engineered barrier: around the waste packages, sealing and backfilling of tunnels and shafts etc. Cement-based materials and clay-based materials are proposed in many repository concepts for backfilling and sealing components in the repository near field.

Experience is based on observations (from laboratory experiments, in-situ demonstration experiments and natural & industrial analogues) supported by interpretative and predictive modelling. This methodology, based on integrating laboratory experiments, field tests, numerical models and natural analogues to up-scale performance in time and space is common practice in radioactive waste disposal R&D and we consider it is advisable to also use this approach to assess the long-term performance of borehole sealing concepts.

A recent report on behalf of RWMD [45] has considered the long-term stability of potential system components for sealing deep investigation boreholes in detail. Almost all information presented in that report is based on programmes undertaken by RWMOs. Only a summary of that report is presented here; the reader is referred to [45] for more information.

5.2.2 Clay-based systems

5.2.2.1 Introduction

Extensive bentonite RD&D programmes are in place at several RWMOs; for example, at SKB, Posiva and Nagra [e.g. 44, 45]. These programmes cover many aspects of bentonite performance. We note that the conditions in site investigation boreholes that will require sealing are often less harsh (for example, in terms of pH or temperature) than those anticipated within the repository near field. Near-field bentonite performance (for example, in terms of maintaining a certain swelling pressure, swelling capacity and low hydraulic conductivity) is evaluated over a much broader range of pressure, temperature and geochemical conditions than those expected in a borehole environment.

It is in this context that the long-term stability of bentonite under conditions similar to those in, for example, the Opalinus Clay (Switzerland), the Callovo-Oxfordian (France) or the crystalline environment (Sweden, Finland), can be assumed to be established. This is illustrated by the feasibility of concepts based on bentonite barriers, as shown by the Entsorgungsnachweis (disposal certificate) in Switzerland [121] or the license application in Sweden (SR-Site). In addition, see recent reviews on bentonite applications for radioactive waste disposal ([122], [123]).

There is, however, a major difference when comparing long-term bentonite performance in the near field of a repository to long-term sealing performance in a borehole. Much larger masses of bentonite would be used to construct near-field engineered barriers than to seal boreholes. This difference may be important if there is a geochemical reaction potential with the host rock that could lead to a potential degradation of the bentonite performance. In a repository environment, it might be acceptable that part of the bentonite loses its performance, using the argument that the remaining bentonite still ensures the performance of the barrier. However, this argument might not be valid in a borehole environment where potentially all emplaced bentonite could be affected by chemical or physical interactions with the host rock.

Chemical interactions between bentonite and other materials placed in the borehole also need to be considered, as they have the potential to result in transformations that might reduce the swelling pressure of the seal material and increase its hydraulic conductivity. The principal interaction to be considered is between bentonite and cement. This and other chemical interactions could take place at the interface between different engineering components, such as between a bentonite seal and the adjacent ‘plug’ component or steel casing. Where seal or plug components are formed of mixtures of materials, changes within the body of the seal or plug also need to be considered. The latter will be more significant because of the much greater surface areas and intimate mixing involved.

A review of the key properties of bentonite and the important processes and issues for consideration in a UK context was produced for RWMD in 2011 [123]. The reader is referred to this reference for detailed information. In summary, the key issues to consider in the context of the current report are:

- onset of bentonite erosion by flowing groundwater (physico-chemical effects);
- chemical interactions between natural groundwater and bentonite. This includes changes both to the swelling capacity of the montmorillonite and mineralogical alteration;
- chemical interactions between bentonite and other components placed in the borehole. The most significant interactions will be with cement, but interactions with steel casing and other metals are also considered.

In the next Sections, key examples of assessing the long-term performance of bentonite engineered barriers and bentonite borehole seals are described.

5.2.2.2 Key experiments assessing the behaviour of bentonite in the repository near field

The FEBEX experiment at the Grimsel Test Site (GTS) consists of an in-situ full-scale engineered barrier system (EBS) test for the disposal of HLW performed under natural conditions [124]. The experiment is based on the Spanish reference concept in crystalline rock in which the canisters are placed horizontally in drifts and surrounded by a clay barrier constructed of highly compacted bentonite blocks. Heating started in 1997 and since then a constant temperature of 100°C has been maintained, while the bentonite buffer has been slowly hydrating in a natural way. A total of 632 sensors were installed in the clay barrier, the rock mass, the heaters and the service zone to measure the following variables: temperature, water saturation, humidity, total pressure, displacement, water pressure.

The experiment was partially dismantled and sampled during 2002. Much of the buffer is saturated and significant swelling pressures have developed close to the rock. The low permeability of the saturated bentonite close to the rock ensured slow saturation and showed that inhomogeneity in rock properties has no influence on buffer saturation. In addition, the buffer inhomogeneity due to construction has played a smaller role than expected and a relatively uniform axisymmetric thermal, saturation and stress response controlled by the distance from the heater has been observed. Density gradients within the buffer have developed due to swelling from the hydration and drying and shrinkage near the heater. In 2015, the FEBEX in situ experiment will be fully dismantled. This will provide a unique characterisation of the key physical properties and chemical properties of the bentonite barrier and its interfaces.

Other examples are the EB test in Mont Terri [125] and the Prototype Repository at the Äspö Rock laboratory [126].

5.2.2.3 Key experiments focussing on bentonite in borehole seals

In order to achieve the design permeability for a bentonite-based borehole seal, the density of the emplaced material needs to be ensured. In addition, the emplacement method should guarantee that no open space is left in the borehole. This consideration is particularly important when assessing borehole sealing longevity because of the small volume of bentonite emplaced, as discussed above. To date, there is little information from experiments on the long-term development of bentonite-based boreholes seals. A summary of available information is given below.

1. The ongoing BOS experiment at the Grimsel Test Site [52] tests the concept for sealing of boreholes drilled from the repository. Sealing elements were emplaced in two boreholes. In BOS 95.001, MX-80 bentonite was emplaced using pneumatic injection; in BOS 95.002, Compactonit® bentonite was emplaced using the MACMET tool. The boreholes were instrumented on either side of the bentonite seals to monitor the development of the bentonite over time and to perform hydraulic testing in the intervals adjacent to the bentonite. The experiment has been in place since 1996; overcoring to assess the bentonite properties is envisaged at some point in the future.
2. Borehole seal experiment as part of project RESEAL [127]. Part of the EC-funded project RESEAL studied the feasibility of sealing off a borehole in the plastic Boom Clay (HADES, Belgium) by means of pre-compacted bentonite blocks. Two bentonites, namely the FoCa and Serrata clay, have been used. Full saturation was reached after five months and was mainly reached by natural hydration. Swelling pressure was lower than originally foreseen due to the slow reconsolidation of the host rock. Later, the efficiency of the seal was tested with respect to water, gas and radionuclide migration. The measured in-situ permeability of the seals was about $5\ 10^{-13}\ ms^{-1}$. A gas breakthrough experiment did not show any preferential gas migration through the seal. No evidence of a preferential pathway could be detected from I-125 tracer test results.
3. The Borehole Plugging Experiment in OL-KR24 in Olkiluoto [46]. Posiva and SKB performed a joint borehole plugging experiment in 2005 in Olkiluoto, Finland. It is described in more detail in Section 4.2.1 of this report.

5.2.2.4 Modelling

Methodologies to assess the long-term performance of near-field bentonite barriers based on modelling are described in detail in [44] and [45] and are therefore not repeated here. Coupled thermo-hydro-mechanical (THM) models can be used to asses the performance of bentonite barriers on timescales beyond the duration of experiments. Nagra [44] envisage that the THM models developed and tested for EBS-related tasks can also be applied to the relatively simpler conditions associated with sealing of site investigation boreholes.

A Jacobs report for RWMD [45] also presents a thermodynamic modelling approach to evaluate the long-term stability of smectites (the principal clay constituent of bentonite). Stability relationships were interpreted using phase diagrams constructed for specific temperatures and compositions of groundwaters that might come into contact with clay-based borehole seals in a UK context.

While thermodynamic modelling can provide insight in the ultimate reaction products and might have a predictive value for certain reactions (e.g. salt dissolution), in general thermodynamic disequilibria are prevailing in nature for many reactions due to the extremely slow reaction kinetics and the formation of intermediate mineral phases, which might be the phases of interest. Kinetic considerations should always be taken into account.

Interactions between bentonite and a range of other engineering materials that might be present in the borehole are discussed in [123]. The processes of bentonite - cement interactions and bentonite – iron interactions are described. Reactive transport modelling to predict the consequences of these interactions has been widely undertaken. Illustrative calculations have been performed as part of this project to illustrate some of the issues, and are presented in Section 6.3 and Appendix 2.

5.2.2.5 Evidence from natural systems

An extensive natural analogue (NA) knowledge base already exists in the context of using bentonite as a material in the EBS of many repository concepts. A major uncertainty, as highlighted in Section 5.2.2.4, is whether smectites would reach thermodynamic equilibrium during the time periods of relevance for post-closure safety. For this reason, quantitative and qualitative evidence from natural analogues has been used to throw light on the long-term stability of clay-based seals in contact with groundwaters. In addition, clay-based materials could be used in close association with other materials in the EBS, such as cements and steels. For this reason, natural analogues have also been used to build understanding of the long-term consequences of these interactions.

A summary of the use of natural analogues in building understanding of the long-term behaviour of bentonite is given below.

Groundwater interaction
Reaction of bentonite in groundwaters of various salinities is of potential concern as very low salinity waters (e.g. glacial meltwaters) may induce erosion and high salinity waters (e.g. brines) may impact on the ability of the bentonite to swell. Other areas of concern include illitisation in high potassium groundwaters which would, once again, impair bentonite's ability to swell. See [128] for a recent overview of the relevant processes.

Fresh water reaction has been examined in several studies (e.g. [129]) and recent work has focussed on examining stability in actual repository sites (e.g. [130]), work stimulated by a review by the Swedish regulator, SSM [131]. Here, the authors noted that smectite occurs at all depths in Forsmark fractures, with no evidence for removal/dissolution by previous glacial episodes. Indeed, smectites have been reported from numerous candidate repository sites in Finland and Sweden that have undergone repeated glacial cycles (details in [128]) with no evidence of chemical or physical degradation.

Seawater reaction with bentonite has been assessed qualitatively in several studies (e.g. [132]). Recent work from the Troodos ophiolite in Cyprus [133] provides new data on the physico-chemical properties of the bentonite for quantitative analysis. At the time of writing, the Cyprus study is unique in NAs of saline water/bentonite reaction insofar that sufficient background information is available to define the time period of reaction (almost 90 Ma), the likely salinity (fully marine) for the vast majority of the bentonite's existence and a range of physical parameters (Natural Moisture Content, Unconfined/Uniaxial Compressive Strength tests, Atterberg Limits (Liquid Limits, Plastic Limits, Plasticity index), Swelling Pressure and Undrained Triaxial Tests), which allow detailed comparison with both laboratory data on saline groundwater/bentonite reaction and on the physical conditions of non-reacted bentonites.

Brine water reaction NA studies are rare (e.g. [134]), but [135] notes some neoformation of smectite in the Wyoming bentonite following reaction with basinal brines at ~2 km depth in Colorado whereas, in Manitoba, neoformation of smectite was also reported following reaction with basinal brines at 20-25℃. The neoformation is evident as fibrous smectite that is concentrated in <0.2 µm fraction and, overall, little or no change is observed in the total smectite content. The presence of smectites at several crystalline sites in Fennoscandia and sedimentary sites in Canada where they have been exposed to brine conditions for several million years was noted by [128], but no examination of the material has been carried out so far.

Illitisation can occur when the flux of groundwater potassium is high enough to cause the montmorillonite to transform to illite, causing loss of swelling potential. This has been studied at great length in the oil industry (see [136] for details) and the boundary conditions (including the crucial temperature range) are well enough documented that the process can be assessed for most future sites. It is recognised that elevated temperatures are required for smectite to illite transformation. The conversion process is complex and displays slow kinetics over a wide range of environmental conditions. Published kinetic models would imply that even in potassium-rich brines (and assuming that potassium supply is not flux-limited) at 50℃ and over 1 Ma, <10% of smectite would be illitized. However, there are uncertainties about these models.

Alkaline reaction with leachates from Ordinary Portland Cement

Bentonite – especially the swelling clay component (smectite) that contributes to its essential barrier functions – is unstable under high pH conditions (Figure 5-1). To assess potential long-term reactions, the Jordan Natural Analogue Study addressed this process at one site, Khushaym Matruk (Figure 5-2) in central Jordan [137]. No other data from NA are currently available to assess smectite behaviour in OPC leachates, but a new project is under consideration by RWMD to look at the reaction between high pH (12-13) cement leachates from the spoil heap of an industrial lime kiln and the underlying natural clays [138]. The maximum period of reaction appears to be 100 years, which would limit the applicability of the study to the longer-term evolution of borehole seal properties.

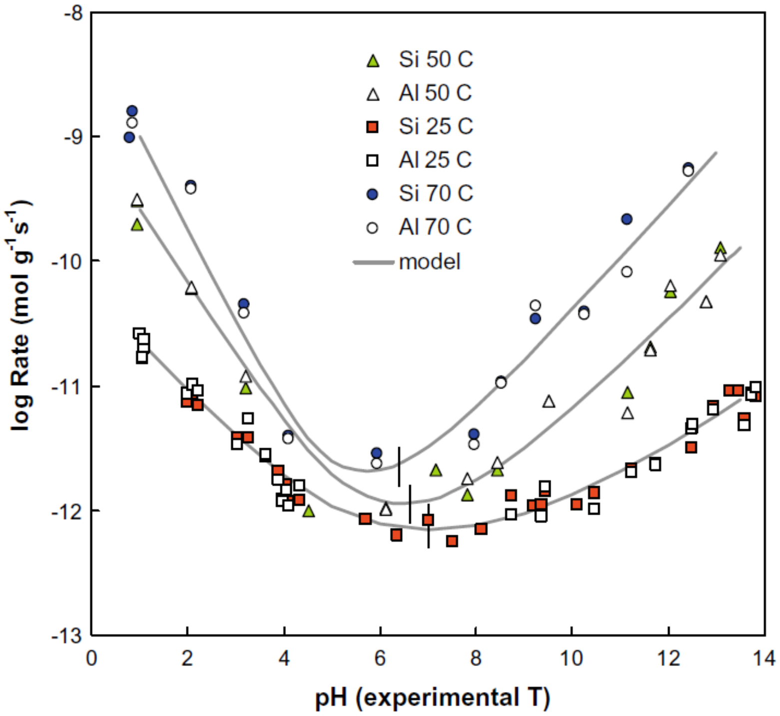

Figure 5-1 pH dependent dissolution rates of aluminosilicates [139]

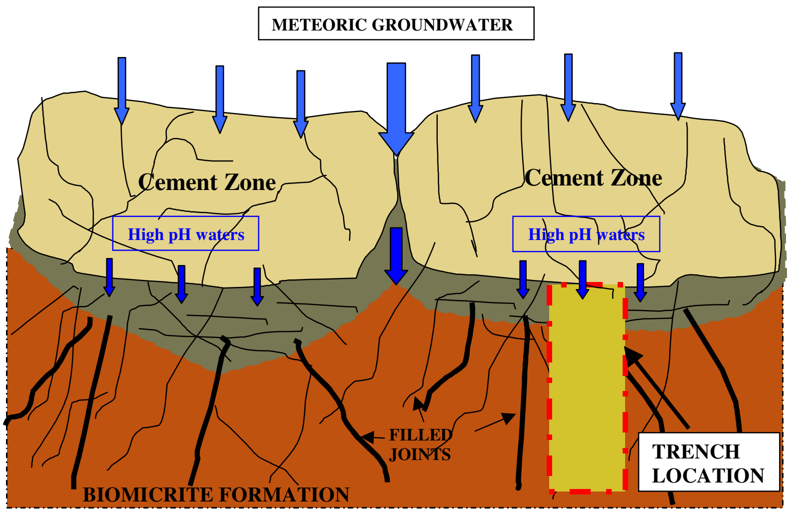

Figure 5-2 Sampling at Khushaym Matruk was by trenching. The trench begins at the cement zone and moves away downslope into the underlying clay-rich sediments. The thermal aureole from the cement combustion extends for the length of the trench [140]

Alkaline reaction with leachates from 'low-pH' concrete
Two recent natural analogue studies, in Cyprus [133, 141] and the Philippines [142], consider the interaction between ophiolite-derived, natural alkali (high pH) groundwaters and bentonite (Figure 5-3). The natural groundwaters are analogous to low-pH cement leachates and the natural bentonites are analogous to the 'industrial' bentonite in the borehole seals. In the case of low-pH cements, it was noted in [10] that a thermodynamic approach to assessing smectite stability found it likely that low alkali leachates would

degrade the bentonite seals. However, these two new NA studies indicate that the lower pH of the leachates (usually pH 10-11) would appear to be less aggressive towards the bentonite.

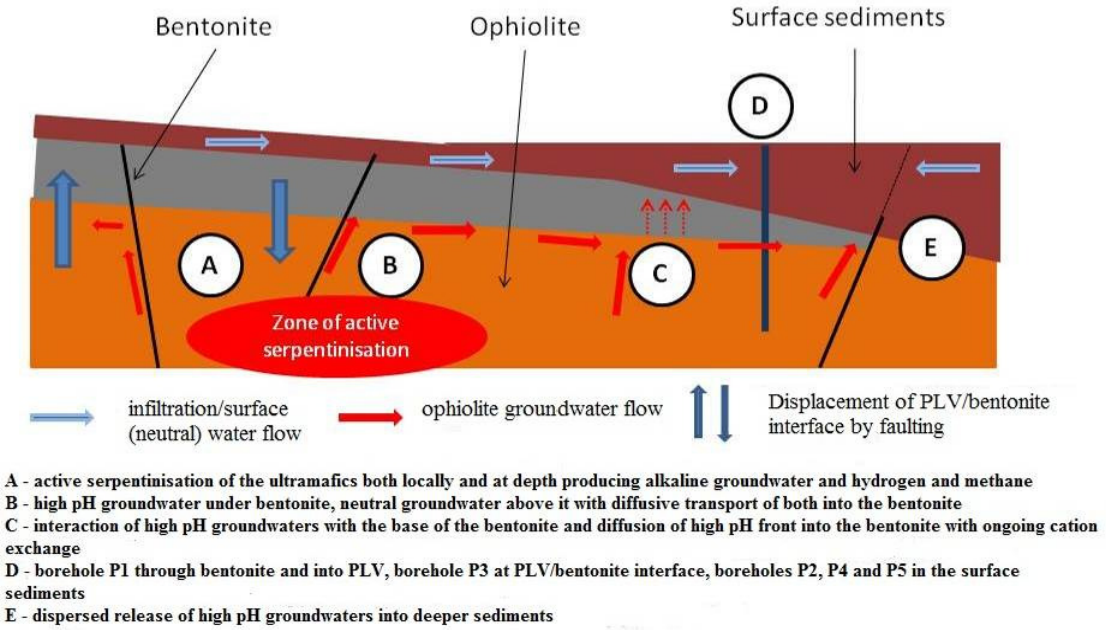

Figure 5-3 Schematic of the Cyprus and the Philippines natural analogues, in which ophiolite-derived, natural alkali (high pH) groundwaters are in contact with bentonite

Although the Philippines NA is at an early stage (see [142] for details), the indications are that reaction in the bentonite is restricted to the contact interface, and the width of the reaction zone is a maximum of 5 mm [143]. In the CNAP study [144], the groundwater appears to have been circulating under the bentonite for some 10^5-10^6 years. In this time, less than 1% of the smectite in the bentonite has reacted to palygorskite, a Mg-rich phyllosilicate, indicating very slow reaction times. A conclusion from the recent CNAP and Philippines studies is that reaction between the leachate and the bentonite appears to be generally driven by diffusive transport of solutes (especially OH and Ca) into the body of the bentonite from the bentonite/alkali leachate contact zone. The physical similarities between the natural bentonite/ophiolite groundwater environment and that expected for the industrial bentonite borehole seals exposed to low-pH cement leachates argue most strongly for limited reaction of the bentonite seals.

Bentonite/borehole steel liner interaction

General observations from natural systems and the NF-PRO URL experiment [145] suggest steel/iron corrosion product could react with bentonite to produce reduced swelling pressure or formation of non-swelling minerals, both of which could impact seal behaviour. Useful NA data are limited (see comments in [146,147]), but potential sites have been identified in [128].

5.2.2.6 Summary of interactions that might affect long-term performance of the bentonite seal

In this Section, we summarise the principal types of interactions that might affect long-term performance of bentonite seals.

Physico-chemical triggers: onset of bentonite erosion
The long-term permeability of bentonite is largely controlled by its swelling pressure. If a significant amount of bentonite is lost from the seal after placement, the barrier would lose its function as a low permeability seal. Depending on the pore water composition and the groundwater velocity in the rock surrounding the sealed section[1], there is a possibility that the bentonite buffer would start to disperse and bentonite colloids be carried away ('eroded') by the flowing water.

The topic of bentonite piping and bentonite erosion is of high importance in the Swedish and Finnish programmes and understanding is currently being developed as part of the BELBaR project[2]. The main aim of the BELBaR project is to increase the knowledge of the processes that controls clay colloid stability, generation and ability to transport radionuclides; the overall purpose will be to suggest a treatment of these issues in long-term safety/performance assessment. In the context of bentonite seals, one of the aims of BELBaR is to understand the main mechanisms of erosion from the bentonite surface and to quantify the extent of the possible erosion under different conditions. The consequences of the onset of bentonite erosion can be bounded for the specific repository conditions of these two countries by taking into account the fracture nature, the flow rate and the anticipated pore water composition at the particular sites being considered. However, a broader understanding is needed should these sealing concepts be developed for other geological environments.

This is especially the case for pure smectite because it cannot currently be demonstrated that it will not erode under certain conditions that might be encountered in the Swedish repository environment. Modelling [148] concluded that for the hydrogeological and hydrochemical conditions encountered in the Swedish disposal concept, the largest fracture transmissivities combined with the highest hydraulic gradients will cause bentonite erosion on the order of 0.3 kg per year for each canister. This is more than one order of magnitude larger than could be reached by smectite particle diffusion alone if fluid flow was neglected. Accessory minerals or adding materials with optimally chosen particle sizes might reduce the risk of erosion; however, this is not yet proven [149]. We note that some of the SKB modelling approaches have been adapted for the fractured rock environment of the Grimsel Test Site (Colloid Formation and Migration Project, Pers. Comm. P. Smith).

Chemical triggers: interactions between host rock porewaters (and host rock) with bentonite
The performance of the sealing element can be affected if there is chemical incompatibility between the host rock groundwater/porewater and the bentonite sealing element. Higher salinity groundwater/porewater in contact with the bentonite has been demonstrated to

1 In the SKB concept, the focus is on groundwater flow in fractures cross-cutting the sealed section. Here, groundwater velocities are substantially higher and pore apertures much greater than in the rock matrix. In disposal concepts involving lower strength sedimentary host rocks or cover rocks, fracture flow is also likely to be the key issue. However, groundwater flow in the matrix of highly permeable strata should also be considered.

2 BELBaR (Bentonite Erosion: effects on the Long term performance of the engineered Barrier and Radionuclide transport) is a project within Euratom FP7: Management of radioactive waste – Geological Disposal. The project reference is 295487.

decrease the swelling pressure (e.g. [150]), and increase the hydraulic conductivity. Especially in very saline waters or brines, this effect can be important. However, no major interactions are expected for less saline groundwater/porewater, such as in Opalinus Clay, Callovo-Oxfordian clay and crystalline basement rocks in Sweden and Finland (but see [128] for discussion). Note that, in these rocks the clay mineralogy is similar to that in bentonite. Other characteristics of the host rock groundwater/porewater that might affect the longevity of bentonite seals are redox state and presence of elevated sulphate concentrations.

Chemical triggers: interactions between cement, high pH pore waters and bentonite
The paragraphs below are largely taken from [44]. These are included here as cement - bentonite interactions are of major importance not only in the 'interface' context as described below, but also when assessing clay - host rock - cement interactions and cement-bentonite mixtures (see further in this Chapter).

Cement-clay interactions have been studied extensively in the last ten years through laboratory experiments, computer simulations and relevant analogue investigations (see [151] for a comprehensive list of references). However, it should be noted that most of these studies have considered the interaction of Ordinary Portland Cement (OPC)-type cement with bentonite, and not formulations of low-pH cements[1]. Taking the lead from these reviews, most authors (e.g. [152]) agree that the most important processes are (see Figure 5-4):

- the interaction of cement/concrete with groundwater will lead to leaching in accord with a sequence of decreasing solubility of cement minerals with time (e.g. [153]);
- diffusive transport of cement pore fluids into bentonite/clay, with mixing and reaction with the clay pore fluids. Sharp gradients in pH (and pCO_2) across the interface encourage the rapid precipitation of carbonates (e.g. aragonite and calcite), and hydroxides (e.g. brucite), leading to decreased porosity (e.g. [154]);
- fast exchange of cations in cement pore fluids (principally K, Na, and Ca) for cations (principally Na+ in MX-80 bentonite) in interlayer sites in montmorillonite, leading to a decrease of swelling pressure. These exchange reactions advance in front of dissolution-precipitation reactions (e.g. [133,155];
- slow dissolution of montmorillonite and other minerals present, such as quartz, feldspars, pyrite, and gypsum. At elevated pH, such reactions consume hydroxyl ions, thus chemically neutralising the advancing cement pore fluids. Multiple reaction fronts form and propagate due to different dissolution and precipitation rates, with later fronts overriding those formed earlier. The overall evolution thus forms a complex porosity structure, with porosity changes within both the concrete and clay. The net change in porosity across the entire alteration zone may be trivial (re-distribution of mass);
- precipitation of secondary minerals such as clays, hydroxides, carbonates, calcium silicate hydrates, and aluminosilicates, such as zeolites and feldspars (e.g. [156]). These minerals may form in a zonal fashion, with relatively more siliceous zeolites more likely to form at lower pH (distal regions of migrating cement pore fluids), whereas C(A)SH, illite, feldspars, and the more aluminous zeolites are more likely to form at higher pH, and hence in the more proximal regions.

Previous studies have highlighted that cement-bentonite interactions are strongly non-linear, with a complex interplay between fluid transport, clay ion exchange and dissolution, secondary mineral growth, and consequent changes in physical properties (porosity, permeability, swelling pressure) of the bentonite. It is also clear that these changes are

[1] See Section 3.7 of [57] for further information on low-pH cement

strongly dependent upon the nature of the cement pore fluid, the type and composition of the bentonite, the mode of fluid transport in the experiment (advection or diffusion), temperature, and time.

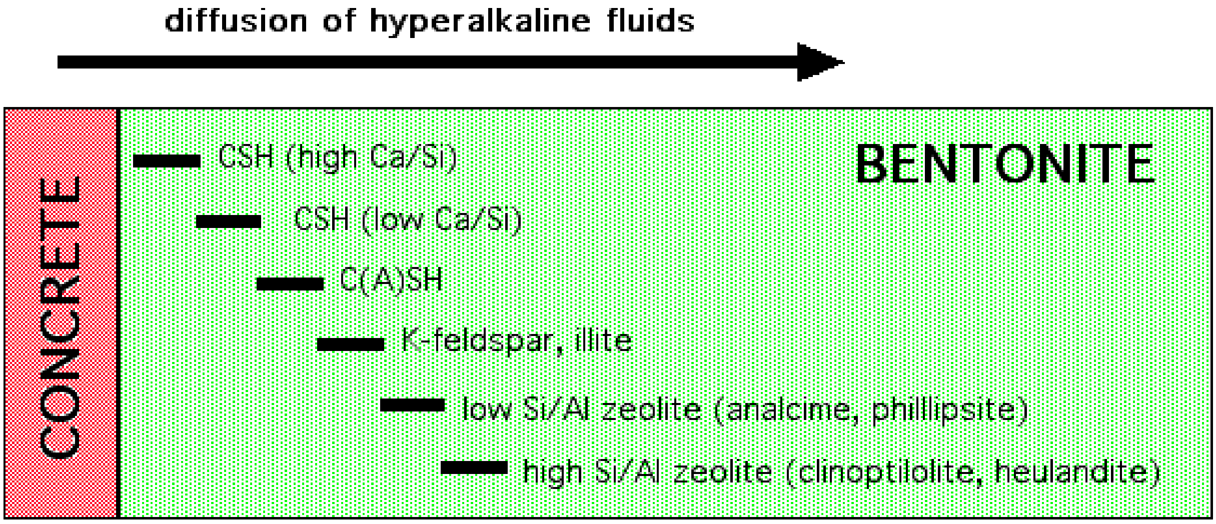

Figure 5-4 Schematic diagram of the potential sequence of secondary minerals due to the migration of (OPC-derived) hyperalkaline pore fluids through bentonite. As the composition of cement pore fluids evolves with time, sodic-potassic phases will be replaced by more calcic varieties. From [156]

Bentonite swelling pressure. Bentonite swelling pressure decreases considerably due to high-pH water interaction, caused by ion exchange and dissolution of montmorillonite (see [157]). The swelling reduction was less (e.g. [158]) or insignificant (e.g. [133]) for low-pH cement compared to OPC.

Hydraulic conductivity of bentonite and diffusion rates. A decrease in swelling pressure and/or bentonite density leads to an increase in porosity and thus to an increase in hydraulic conductivity (e.g. [159]) and diffusion rate (e.g. [160]). On the other hand, evidence from laboratory and analogue data shows strongly reduced porosities in the bentonite or clay due to mineral precipitation a few mm to cm away from the cement-clay contact (e.g. [151], [161])[1]. These findings can be well reproduced by modelling. As a consequence, a decrease in hydraulic conductivity across the interface can be expected. It is further documented that diffusion rates of bentonite and clay rock decrease due to high-pH interaction [162]. Note that these observed and modelled reductions in hydraulic conductivity and diffusion rates are across the cement-clay interface and thus governed by the low porosity zone consistently detected.

In a borehole sealing context, these types of interactions are expected to occur at the interface between two elements of the sealing system and to be limited by diffusion as the dominant transport mechanism. In this case, where diffusion is the driver and the reactive surface area between the two materials is relatively small, the extent of the zone affected is expected to be small, of order of a couple of centimetres over long timescales. Although these reactions will occur irrespective of the original purpose of the borehole,

[1] Note that these observations are for OPC. No such changes were seen in the Cyprus or Philippines analogue studies, where the high pH fluids are analogues of low alkali cement leachates

their relevance is more prominent for radioactive waste disposal because of the long required lifetimes of post-closure seals.

5.2.3 Cement-based systems

5.2.3.1 Overview

Cementitious materials are included in the designs for all current concepts for geological disposal of higher activity wastes worldwide [57]. Cements are envisaged being used in a wide range of applications: as waste encapsulation grouts; waste containers and overpacks; buffers and backfills; fracture grouts; tunnel plugs; tunnel/vault linings, floors and roadways. These uses of cement materials range from those related to operational safety through to those related to post-closure safety. The safety functions of the cement material depend on the application, but include its mechanical strength, its capacity for maintaining a high pH environment and its sorption capacity towards radionuclides.

The varying applications of cements in the EBS of a GDF place a wide variety of performance requirements on the materials used. As a result the cement materials under consideration differ significantly in their formulations and in their chemical and physical properties. In the context of borehole sealing, we are principally interested in mechanical stability (the ability of the cement-based material to support overlying sealing elements and minimise any displacement). Sealing performance (as measured by permeability) is also an issue in some circumstances.

5.2.3.2 Optimisation of cement-based materials for sealing

A recent report for RWMD, produced by Serco in 2012 [57], gives the current status of cement materials for use as sealing materials in geological disposal concepts. Only high level conclusions from this report are given here. The reader is referred to [57] for further information.

The scale of sealing applications of cements in GDF concepts ranges from the tens of microns for fracture sealing grouts to the 1-10 metre scale for transverse tunnel and drift plugs [57]. These differences in scale place differing requirements on the cement formulations. Fracture sealing grouts have specific requirements for penetrability into fractures and minimal bleed and are made from so-called micro-cements (with finer particle size than conventional cements); tunnel plugs are made from concrete, and due to their large mass, minimisation of temperature excursions from cement hydration becomes an important criterion.

For disposal concepts that include a clay-based buffer, low-pH cements are the preferred option for waste disposal areas. Low-pH cement fracture-sealing grouts have therefore been developed by SKB and Posiva and have been extensively tested at ONKALO and through the ESDRED Project. Low-pH concretes have also been developed for tunnel seals and plugs. A number of prototype designs of tunnel plugs constructed from different concrete formulations have been tested successfully in underground research laboratories through international programmes (e.g. TSX, FEBEX and ESDRED).

5.2.3.3 Longevity

Cement is thermodynamically unstable in essentially all environments relevant to borehole sealing. Foremost amongst the changes that will occur is the evolution with time and temperature of the metastable phase, the C-S-H gel binder, which typically comprises >50% by mass of Portland cement. In barrier applications with intended performance lifetimes in the range of a few hundred years, evidence from historical cements (summarised below) that have not been subject to thermal excursions, suggests that CSH will persist. Experience and computer models can also be used together to yield defensible predictions of cement cracking, strength, and permeability for cements exposed to typical (near-surface) environments for at least 50 to 100 years or possibly a few hundred years [163]. Recent developments in concrete science claim that '*a containment vessel for nuclear waste built to last 100 years with today's concrete could last up to 16,000 years if made with an ultra-high-density (UHD) concrete*' [164].

Ultimately however, CSH will crystallise [165] and the chemical and physical properties of the cement will substantially change. Consequently, whilst there is a good understanding of the properties of cement-based barriers over timescales relevant to conventional engineering applications (tens to hundreds of years and, potentially, up to thousands of years), important uncertainties persist about its properties over longer timescales relevant to the post-closure performance of a geological disposal facility. Indeed, RWMOs generally assume that little or no credit can be taken for cement as a long-term low permeability barrier in the EBS.

In addition, as discussed in Section 5.2.2, cement-based seals may have detrimental effects on the performance of adjacent clay-based seals and rocks, principally through creating a high pH environment and thereby inducing a range of short-term and longer-term chemical reactions. The use of low-pH cement might limit this impact. In this context, the Serco report [57] concludes '*The immediate consequences of using low-pH concrete formulations are largely beneficial. However, the longer term consequences of using large quantities of slowly reactive aggregates such as silica fume and fly ash are not well understood. For example, the mineralogy, and with it the physical properties and pH-buffering behaviour, may change, but the extent and direction of change are not yet known'.*

5.2.3.4 Evidence from analogues

Ordinary Portland Cement
The natural cements at Maqarin, northern Jordan were formed by the combustion of organic-rich limestones, a process which continues today [166]. The oldest reported cements in this area are some 2 Ma old [167] and reaction is very much restricted to the edge of fractures. This is possibly because the natural material is of low porosity and permeability and the secondary reaction products naturally seal any flowing porosity [140]. The presence of unreacted natural cements have been reported from the Scawt Hill and Carneal Plug sites in Northern Ireland [168]. These phases were produced during the thermal metamorphism of the host limestone and are estimated to be some 58 Ma old. As with the cements in Jordan, these natural cements in Northern Ireland remained unchanged until accessed by groundwaters in the last 10-20 ka [169].

These are the only two sites where OPC cement longevity has been studied in any form and then very much as secondary objectives. It appears that, in both cases, the cement has survived due to self-sealing of the reaction pathways. In both sites, this is from the secondary products (CSH, CASH, zeolites etc at Maqarin, carbonates at Scawt Hill and Carneal) formed during the cement leaching. However, to be able to make any meaningful observations on the likely longevity of OPC concrete borehole seals, it would be necessary to re-examine the sites with this objective as the focus of the study.

Low-pH cement
Low-pH cement is essentially the same as the pozzolanic cements developed by the Romans in the 3rd century BC. The Romans particularly used the pozzolan cements in positions where it was important to prevent the penetration of water or damp, such as lining water channels and tanks. The cement also offered good resistance to seawater and so was used extensively for Roman marine structures. Importantly, as noted in [170] *'It is remarkable that these observations made by Vitruvius about 16 BC, almost 2000 years ago, compare so well with those in modern specification or code of practice'* suggesting that the ancient Roman pozzolanic cements are an appropriate analogy for the low-heat cements proposed for use as borehole seals.

Work (e.g. [171]) is currently ongoing by the ROMANCON (Roman Maritime Concrete Study) group looking at a wide range of sites around the Mediterranean (Figure 5-5). Unfortunately, only preliminary data are currently available from the ROMANCON studies. Further analyses to investigate microstructural variability, related to different stages of dissolution and precipitation, is *'ongoing'* [172], so it is currently difficult to assess if seawater immersion for two millennia has had a deleterious effect on the Roman low-heat cements. As a minimum, all of the ROMANCON authors point out the incredible condition of the concretes examined so far and admire their obvious durability in such an aggressive environment.

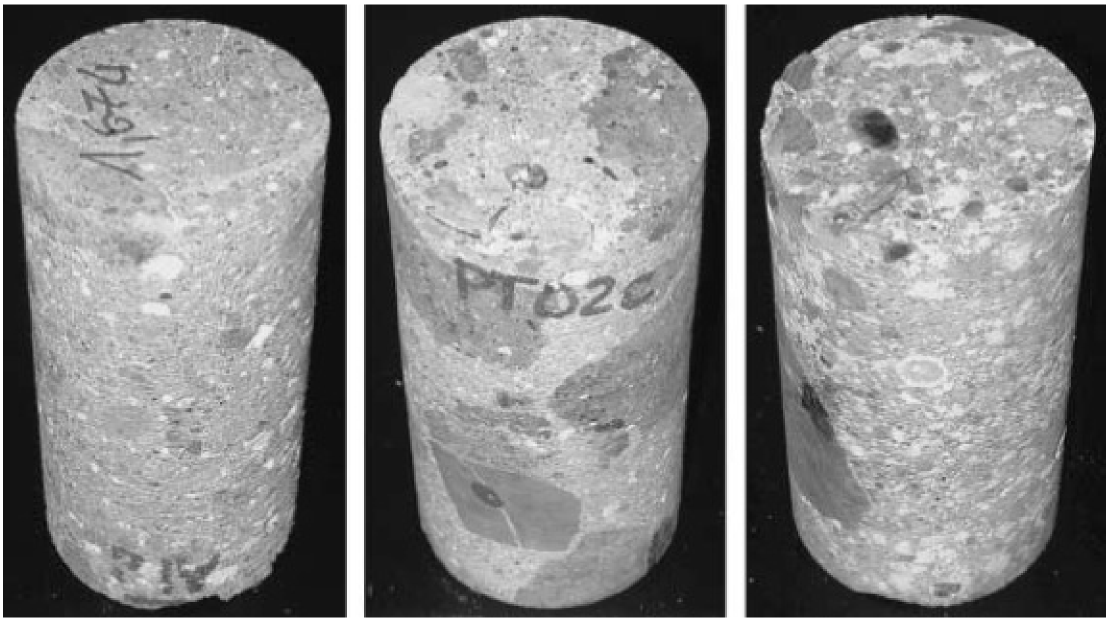

Figure 5-5 Typical core samples recovered from sites at Portus and Anzio [171]

5.2.3.5 Bentonite/cement mixtures

The chemical incompatibility between cement and bentonite is extensively described in Section 5.2.2. By mixing bentonite and cement in a single seal, the surface area over which these reactions take place is increased by orders of magnitude compared to the surface area of a single interface between a bentonite-based seal and a cement-based seal. A high ratio of surface area to volume results in an increase in reaction rates, and consequently speeds up the rates at which the mineralogy of the bentonite and cement fractions change and the performance of the seal degrades.

Therefore, although bentonite/cement mixtures are commonly used for sealing boreholes in other applications (e.g. sealing to protect water resources), they have not been considered in any detail as post-closure seals. The fact that long-term performance is an essential condition for such seals is likely to be the reason for this.

5.2.4 Evaporites

5.2.4.1 German programme

As noted in Section 4.2.3, there is a lack of publicly available information from the German research programme into borehole sealing in evaporites. However, GRS has published the results of its experiments in the Asse mine investigating the long-term evolution of crushed salt backfill in 60 cm diameter disposal boreholes [64]. Of most relevance to the sealing of site investigation boreholes is the DEBORA 2 experiment focusing on the region above the canister stack, rather than between the canisters and surrounding rock (DEBORA 1).

During the 15 months of the experiment, a maximum temperature of 135°C was achieved through electrical heating, and a maximum backfill pressure of ~15 MPa was measured. The convergence-induced borehole closure was 42.5 mm, with a corresponding decrease in porosity (from 37 % to 12 %) and permeability (from 1 10^{-10} m^2 to 4 10^{-13} m^2)[1]. The final permeability was still high compared to measurements made in undisturbed rock salt in the Asse mine (<10^{-21} m^2), and the authors questioned whether such values could be achieved by simple compaction of crushed salt [64]. There was good agreement between the measured and predicted behaviour, particularly for the long-term compaction rates (<0.05 mm per day) reached in the final stage of the experiment.

5.2.4.2 WIPP

Representative mechanical properties after 28 days, 90 days and 1 year for the saltwater grout and expansive salt concrete described in Section 4.2.3 give an indication of the post-emplacement evolution of these materials (Table 5-1) [67].

Table 5-1 Representative mechanical properties of seal materials used in field tests

	Saltwater Grout			Salt Concrete		
	28 days	90 days	1 year	28 days	90 days	1 year
Unconfined compressive strength (MPa)	49.6	68.0	82.0	31.0	34.5	47.5
Static modulus of elasticity (10^3 MPa)	13.1	20.0	20.7	20.7	24.1	32.4
Restrained expansion (%)	0.05	0.11	0.38	0.09	0.13	0.21
Permeability to brine (10^{-18} m^2)	<1.0	1.0	1.0	<0.8	0.8	0.8

Samples of the expansive salt-saturated concrete and grout that had been emplaced in 1985 and 1986 were recovered for analysis in 1991, and the material was found to have maintained its physical and compositional integrity in spite of exposure to brine [173]. WIPP researchers have noted that the long-term (500-1000s of years) performance of grout and concrete seals is less predictable than that of a natural halite plug, and this is another reason for considering a combined seal [69].

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[1] Permeability k is a function of the medium only and has dimensions L^2. The permeability k and hydraulic conductivity K of a porous medium are related in the following way: $K = k\rho g/\mu$, where the fluid density ρ and the dynamic viscosity μ are functions of the fluid alone and g is the acceleration due to gravity. Hydraulic conductivity specifically refers to the ability of the medium to transmit water. At 20°C, the conversion factor is $1 m^2 = 1\ 10^7\ ms^{-1}$.

5.2.4.3 Evidence from analogues

In the German programme, previous NA work focused on tunnel backfill and other material properties (e.g. [174]) or on the far-field retardation of radionuclides (e.g. [175]). More recently, the ISIBEL-I and ISIBEL-II projects (on the applicability of NAs for the safety assessment of repositories in salt) have looked at potential NA for a much wider range of processes and materials (see [176, 177] for an overview). These projects have identified potential NA studies to cover such areas as the long-term stability of bentonite as a seal in rock salt, the long-term behaviour of cementitious materials in salt and long-term compaction of rock salt backfill.

5.3 Experience from oil and gas industry

5.3.1 Scope of testing and validation for seal materials

The main characteristics sought from barrier materials for PA of oil and gas wells are:

- pumpability, or other ease of emplacement;
- setting/settling characteristics that will minimize rig-time;
- very low permeability;
- non-shrinking;
- ductile, non-brittle;
- ability to bond to casings and/or formations;
- resistance to downhole fluids and gases;
- long-lasting performance and isolation characteristics.

The deployment of seal materials follows a sequence of development, qualification, installation and verification. In terms of their pumpability or placeability, the desired characteristics are designed into the materials at their development stage, and their properties and behaviours are verified through laboratory testing. In the field, as part of the preparation for emplacement, characteristics such as slurry densities and viscosities are monitored and measured at the rig site to ensure the materials are placeable as designed. Where required, adjustments (within specified permissible limits) are made to the mixes to achieve the required characteristics, and if these are not met then the material is discarded without being emplaced.

In the case of hardened cements or other materials emplaced around casings, properties can be inferred from log techniques (acoustic, pulsed neutron, resistivity). However, these are indirect measurements, intended primarily to detect channels, heterogeneities and pore bonding, and they do not provide direct determinations on material properties as might be needed for QC purposes.

Theoretically, it would be possible to sample cement seals after they had hardened and to determine their properties. However, as this would involve re-entering the well with a coring assembly or taking rotary side-wall cores through the casing, this is rarely if ever undertaken. The question would also arise as to how representative any cored sample might be, unless it was taken some distance from the bottom or top of the emplaced plug at a depth where there was no potential contamination from other borehole fluids. Attempts to downhole sample emplaced non-setting materials would only result in a disturbed sample being returned to surface.

Likewise, there is no opportunity to test the evolution of any materials once they are emplaced, given that the well will be closed and abandoned and the rig moved before any meaningful ageing of the materials might take place. This is in contrast to the situation in backfill of a large mine opening or engineered vault, where tests might be performed on emplaced sealing materials in situ, or where there might be access to conduct rigorous and controlled sampling of emplaced materials for testing back in a laboratory.

Therefor2e, once seal materials are emplaced in an oil or gas well, it is only overall seal integrity or the integrity of individual components that is measureable downhole (via pressure tests, see Section 4.3.8) and not any intrinsic material properties or characteristics. This means that any material tests are limited to those performed at the qualification stage of the process (during and immediately after product development), or as part of a QC procedure using things like hardened cubes or cylinders prepared at surface using slurries collected during the mixing and placement operations at the rig-site.

5.3.2 Laboratory tests for seal material qualification

Worldwide, the laboratory testing programmes used to assess potential seal materials for oil and gas PAs are left largely to the discretion of the oil companies (the larger ones of which have their own internal standards for all aspects of PA), and the researchers and manufacturers of the materials themselves. State and national rules and guidelines make little or no reference to material specifications other than in the broadest terms. One exception to this is the UK, where a detailed document has been published specifically on the topic [80][1]. This includes detailed guidelines on which tests are relevant, what properties should be assessed, and some minimum standards that need to be achieved.

In these guidelines, the potential materials for PA are grouped into nine material types, with the following three types being most relevant to RWMD:

- Type A – Materials that set solid (i.e., cements, Pozzolan mixes, hardening ceramics);
- Type B – Non-setting grouts and slurries (i.e., sand or clay mixtures, bentonite pellets, barite, and inert particle mixes;
- Type F – Natural formation (i.e., claystones, shales, salt);
- Type I – Metals.

The remaining five material types are gels, composites, thermoplastics, polymers and glass.

For each of the material types, mandatory and recommended tests are defined for the evaluation of a range of properties associated with:

- Permeation;
- stability to fluids;
- dimensional stability;
- mechanical properties (including deformabilities, strengths and creep).

[1] The reference has been developed specifically for the UK, by the UK operators in consultation with the UK regulatory authorities. However, as probably the most complete set of guidelines on this subject within the industry, it has been adopted (or at least sections of it have been adopted) by many of the international oil companies as setting their internal standards for their worldwide operations.

These UK guidelines also reference a number of test standards and suggested methods, largely from those of:

- British Standards Institute/ISO;
- ASTM (American Society for Testing and Materials);
- International Society for Rock Mechanics (ISRM).

For full details of the suggested test programmes and parameters to be determined to assess wellbore sealing materials for PA, refer to the full document [80]. However, as an introduction to the guidelines on those materials types most relevant to RWMD's sealing concepts, see Table 5-2, Table 5-3 and Table 5-4.

Property		Requirement	Test	Ageing required	Before ageing	After ageing
PERMEATION						
Permeability to water		Mandatory	Constant head or decay pulse at 20°C	Yes	<0.25 m^3/year	<50% increase
FLUID STABILITY						
Dry mass		Mandatory	Oven drying at 105°C	Yes		<3% loss
DIMENSIONAL STABILITY						
Expansion or swelling	During hardening	Mandatory	ISO 10426 ring-test		<1% by volume	
	When hard	Mandatory	ISO 10426 ring-test	Yes		<1% by volume
Shrinkage	During hardening	Mandatory	ISO 10426 ring-test		<1% by volume	
	When hard	Mandatory	ISO 10426 ring-test	Yes		<1% by volume
Differential thermal expansion		Mandatory	ASTM E228		<1% linear strain difference	
Creep		Mandatory	ASTM C512-10		<1% linear strain	
MECHANICAL PROPERTIES						
Elastic	Young's modulus	Recommended	ASTM C469	Yes		
Strength and hardness	Tensile Strength	Mandatory	Brazil test ASTM C496	Yes	>1 MPa (145 psi)	>1 MPa (145 psi)
	Uniaxial compressive strength	Mandatory	ISO 10426-2	Yes	>1.4 MPa (200 psi)	>1.4 MPa (200 psi)
	Hardness	Recommended	ASTM E384	Yes		
	Shear bond strength	Mandatory	Extrusion from steel tube (ASTM D7127 for internal rugosity of tube)	Yes	>1 MPa (145 psi)	>1.4 MPa (200 psi)
OTHER CHARACTERISTICS						
Bulk density		Recommended	ASTM C138	Yes		

Table 5-2 Guidelines for laboratory qualification of cements and other setting barriers for PA of UK oil and gas wells as given in [80]

Property		Requirement	Test	Ageing required	Before ageing	After ageing
PERMEATION						
Permeability to water		Mandatory	Constant head or decay pulse at 20°C	Yes	<0.25 m^3/year	<50% increase
FLUID STABILITY						
Dry mass		Mandatory	Oven drying at 105°C	Yes (depending on material)		<3% loss
DIMENSIONAL STABILITY						
Expansion or swelling	During hardening					
	When hard					
Shrinkage	During hardening					
	When hard	Mandatory	ASTM D4943	No	<0.4% by volume	
Differential thermal expansion		Mandatory	ASTM E228		<1% linear strain difference	
MECHANICAL PROPERTIES						
	Shear bond strength	Recommended	Extrusion from steel tube (ASTM D7127 for internal rugosity of tube)	Yes	>1 MPa (145 psi)	>1.4 MPa (200 psi)
OTHER CHARACTERISTICS						
Bulk density		Mandatory	Pressurized mud balance			

Table 5-3 Guidelines for laboratory qualification of grouts and non-setting solid barriers for PA of UK oil and gas wells as given in [80]

Property		Requirement	Test	Ageing required	Before ageing	After ageing
PERMEATION						
Permeability to water		Mandatory	Constant head or decay pulse at 20°C	Yes	<0.25 m^3/year	<50% increase
FLUID STABILITY						
Dry mass		Mandatory	Oven drying at 105°C	Yes		<3% loss
DIMENSIONAL STABILITY						
Expansion or swelling	When hard	Recommended	ISRM			
Shrinkage	When hard	Recommended	ISRM			
Differential thermal expansion		Recommended	ASTM E228			
Creep		Mandatory	ASTM C512-10	Determined by application		
MECHANICAL PROPERTIES						
Elastic	Young's modulus	Recommended	ASTM C469	Yes		
	Poisson's ratio	Recommended	ISRM			
Strength and hardness	Tensile Strength	Recommended	Brazil test ASTM C496	Yes		
	Uniaxial compressive strength	Recommended	ISRM	Yes		
	Cohesion	Recommended	ISRM triaxial test	Yes		
	Friction angle	Recommended	ISRM triaxial test	Yes		
	Hydrostatic compressive yield	Recommended	ISRM triaxial test	Yes		

Table 5-4 Guidelines for laboratory qualification of formation rocks as suitable materials for PA of UK oil and gas wells as given in [80]

5.4 Experience from CO_2 storage

5.4.1 Introduction

In Europe, CO_2 storage projects will be regulated in fulfilment of the requirements of the European Commission's Directive on Storage [178]. Effectively this means that an operator of a CO_2 storage site must show that there is an insignificant risk of CO_2 leakage and that CO_2 will be contained permanently; it follows that all available evidence must show that seals in wells associated with CO_2 storage must never fail.

Notwithstanding the above, the timescales for which CO_2 will need to be retained underground are not precisely defined. Owing to the long residence time of CO_2 in the atmosphere, storage must be effective for at least several thousands of years if climate change is to be mitigated. Thus, the developing CO_2 storage industry must assure regulators that borehole seals will be effective over at least this timescale.

The methodologies and the modelling strategies into seal longevity are of high relevance in the current context as this is recent ‘state of the art’ work in an area with many similarities to radioactive waste disposal. However, it is important to recognise that supercritical CO_2, whilst itself relatively unreactive with respect to borehole seals, dissolves in formation water to produce an acidic solution. Such conditions are not directly relevant in the context of radioactive waste disposal although, as discussed below, such conditions will be more aggressive towards cement than the near-neutral groundwater pH conditions that would be encountered in site investigation boreholes constructed around a GDF.

Considerable research has been undertaken to investigate the reactions that may occur between CO_2-charged formation waters and borehole seals. This research has built confidence that boreholes in CO_2 storage projects can be sealed effectively. The experience is relevant to post-closure borehole seals at a site for a GDF because it helps demonstrate that seals can be effective under in-situ environmental conditions that are more aggressive towards cement seals than would be encountered within a GDF and surrounding rocks. Not only are seals in CO_2 storage sites exposed to more reactive fluids, but also they may be at considerably higher temperature than would be encountered in the environs of a GDF. In a CO_2 storage reservoir, it would not be unusual for the temperature to be in excess of 100 °C, in contrast to a GDF where most likely the temperature would be <50 °C (Section 3.3.5).

DNV led a consortium of energy companies to develop a risk management framework for existing wells at potential CO_2 storage sites termed “CO2WELLS” [179]. This guideline included a recommendation to assess well integrity risks, including the failure modes illustrated in Figure 5-6. Corrosion of carbon steel pipe and cement degradation were considered to be the most likely long-term seal failure mechanisms, although the actual probability of failure would depend upon the rate of corrosion and cement degradation.

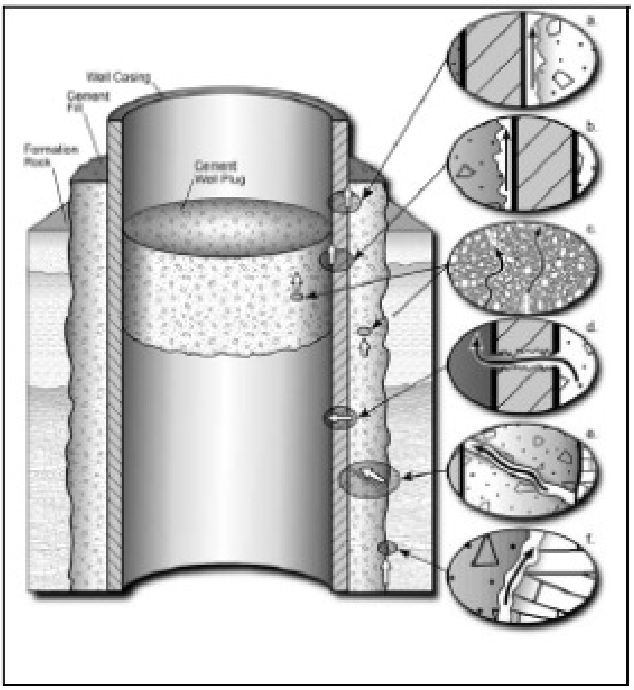

Figure 5-6: Schematic illustration of possible CO_2 leakage pathways through a well (after [180]). a) between cement and outside of casing; b) between cement and inside of casing; c) through the cement; d) through the casing; e) through fractures in cement; and f) between cement and formation.

5.4.2 Laboratory experiments to evaluate seal longevity

Several experimental studies have been undertaken to investigate the longevity of borehole seals in the presence of CO_2 (e.g. [181], [182], [183] [184], [185], [186]). These experiments have involved reacting cement and / or steel samples with CO_2/CO_2-charged water in batch or flow-through systems.

These studies have included investigations of reactions between the major cement ingredient portlandite ($Ca(OH)_2$) and CO_2 or CO_2-charged water (e.g. [182], [186]). Batch reactions between portlandite samples and supercritical CO_2 at a pressure of 160 bar and temperatures of 80, 120, and 200 °C, both with and without liquid water being present, were reported by [182]. Examination of the reaction products by scanning electron microscope showed that when liquid water was present, the portlandite was completely carbonated to form calcite. In contrast, when liquid water was absent the portlandite was incompletely altered owing to the surfaces of the portlandite crystals being passivated by coatings of small calcite crystals.

Rochelle and Milodowski [186] compared the results from carbonation experiments of Portland cement with the carbonation of natural cements found in the aureoles of igneous intrusions in Northern Ireland. Experimental and natural samples were found to have very similar carbonation characteristics even though the conditions of carbonation had evidently taken place under very different conditions and over very different timescales (the natural samples possibly having been carbonated over a period of several thousand years). In both the experimental and natural samples CSH phases observed found to have been transformed to $CaCO_3$ and SiO_2, and there were well-defined reaction fronts between unaltered and carbonated material. In the laboratory samples, localised Ca migration and matrix porosity increases were identified at the reaction front. There had been localised shrinkage of the cement matrix with concomitant cracking. However, a zone of $CaCO_3$ precipitation behind the reaction front partly sealed porosity. It was found that the reaction zone was broader and more porous / permeable in the experiments than in the natural samples, implying that the short-term experiments might not reproduce the longer-term much slower processes that would occur in an actual seal. Possibly the more limited carbonation of natural samples, even over the very long timescales for which they had been exposed to atmospheric CO_2 or dissolved HCO_3^- in groundwater, could reflect armouring of CSH phases by relatively limited amounts of calcite precipitation.

There is some experimental evidence that the resistance of the cement to CO_2 attack depends upon the conditions under which the cement cures. Kutchko et al. [181] found that cement cured at 50 °C and 30.3 MPa (representing the conditions in a CO_2 storage reservoir) was more resistant to reaction with carbonic acid than cement cured at 22 °C and 0.1 MPa. Samples of the former cement were degraded to shallower depths and showed a more well-defined carbonated zone than the cement cured under ambient conditions. The greater resistance of the cement that was cured at higher temperature was attributed to $Ca(OH)_2(s)$ crystals being more evenly distributed, thereby forming a more uniform and effective barrier to CO_2.

Carroll et al. [184] report batch experiments on cement and cement-bentonite mixtures, based on materials used to complete wells in the demonstration CO_2 storage site at Krechba, Algeria. These researchers used a powdered class G oil well cement. In the experiments with bentonite, the bentonite to cement ratio was 1:39 by weight, reflecting mixtures identified in well logs from Krechba. However, they did not report the outputs from these experiments in a form that allows comparison with experiments that used only cement. Reactions used synthetic brine and supercritical CO_2 at 95 °C and 115 °C and 10 MPa. They found that the observed mineral transformations could be explained by a relatively simple geochemical model. Dissolved Ca was explained by portlandite and CSH carbonation, whereas brucite and hydrotalcite dissolution controlled dissolved Mg. The Si released from the cement through carbonation was thought to be incorporated into precipitated chalcedony. Nevertheless, Si and Ca concentrations were buffered at sufficiently high levels to cause smectite to precipitate in both the cement - sandstone and cement - shale experiments. An important finding was that dissolved Mg, which is an important constituent of many formation brines, can react with cement to form poorly-crystalline solids. These researchers considered that further research was needed to assess the impact of the Mg - induced alteration on wellbore integrity.

Carey et al. [183] investigated the flow of a 50:50 mixture of supercritical CO_2 and saline water (30,000 ppm NaCl) through a simulated sealed borehole, consisting of a casing and a Portland cement plug, at 40 °C and 14 MPa pore pressure for 394 hours. Approximately 59,000 pore volumes of fluid moved through the casing–cement grooves. They found very little evidence for mass loss from the cement, but the steel casing corroded to a depth of 25-30μm and calcium and iron carbonate precipitated within channels that formed in the steel.

5.4.3 Field experimental investigations

Field experience provides some evidence for the likely behaviour of well seals in the presence of CO_2 over longer times than have been examined in laboratory experiments, although still over much shorter times than those for which CO_2 must be stored ([187], [188], [189]).

Observations on borehole casing, cement and wallrock samples recovered from a well in the Scurry Area Canyon Reef Operators (SACROC) oilfield in Texas provide the longest-term evidence available ([187], [189]). The SACROC reservoir is situated in the Permian Basin of West Texas and is the second oldest continuous operation to Enhance Oil Recovery (EOR) by CO_2 flooding in the world, having been operated since 1972. The CO_2 flooding has recovered 38% of the injected CO_2 for re-injection; the rest, some 68 million tonnes is effectively sequestered. The temperatures and pressures in the SACROC reservoir average 54°C and 18 MPa respectively.

The investigated SACROC well was drilled in 1950 and first produced CO_2 in 1975 to recover CO_2 that had been injected via other wells. This production lasted for 10 years, after which the well was used to inject 110,000 tonnes CO_2 over a period of a further seven years. The well has therefore been exposed to both low and high pressure environments, corresponding to CO_2 recovery and injection respectively. During the production period the well probably interacted with less pure CO_2 than during the injection period, when the environment close to the well was more CO_2-rich. While production was occurring the well may have been exposed to acidic carbonated water that would have been particularly reactive with respect to the cement components of the well. During the years after the well was operated, the remaining CO_2 near the well probably interacted with the formation fluids to produce another less pure CO_2 fluid, which may have then continued to react with the well cement.

The precise composition of the cement used to seal the well is unknown, being described in the logs as simply ‘Portland’. However, Carey et al. [187] assumed that the cement was neat Portland cement (specifically with no bentonite gel additives), with a density of 1857 kg m^{-3} and described it as being ‘Ca rich, Si-poor’. In 2006, a 5 cm side-track core sample was taken from the well. The sampled material extended from a depth of 1,994m to the shale-limestone reservoir contact at 2,000 m. Samples of casing and cement were retrieved in the first two metres, with shale being collected in the remaining four metre section down to the contact with the reservoir.

The observations showed that geochemical alteration occurred along cement-casing and cement-rock interfaces, with little alteration extending deeper into the cement core. At the former interface there was a dark rind (0.1-0.3 cm) between the casing and the cement whereas at the cement-shale interface an orange alteration zone (0.1-1 cm) occurred. The dark rind was found to be composed of $CaCO_3$ (both calcite and aragonite) and the component of amorphous material was insignificant. The orange zone was found to be heavily carbonated cement and to consist of the $CaCO_3$ polymorphs calcite, aragonite and vaterite, together with a large quantity of amorphous material. Both zones were observed to contain halite. However, the overall integrity of the cement's structure was found not to have been compromised in either zone and there was no evidence for the permeability of the altered zones being significantly less than that of the fresh cement. The casing steel was also found to be in excellent condition, from which it was concluded that the alkaline chemical environment maintained by the cement had prevented corrosion. Thus, the cement and steel together provided an adequate flow barrier for the 55 years that they have been in the reservoir. Since the examined well components were located 3-4m above the reservoir contact, it can be concluded that at higher levels in the well, the cement seal would be even less affected by the action of CO_2.

Crow et al. [188] report a similar study to the one reported by [187], except that the investigated well was a CO_2 producing well that exploited a natural CO_2 accumulation in the Dakota Sandstone of the central U.S.A. The well had a barrier system that comprised a 7-inch diameter carbon steel casing cemented with a Portland cement- fly ash mix. The cement was Class H, with 50% fly ash and 3% bentonite gel. As in the SACROC well, samples of the well casing and cement were taken by sidetrack drilling. It was found that, as at the SACROC site, cement carbonation had occurred. This carbonation had caused increased permeability and porosity, a small increase in capillary entry pressure and a decrease in compressive strength. However, the cement still functioned as an effective barrier. The casing was also found to be in very good condition, probably due to high cement coverage and little flow of reservoir fluids along the casing-cement interface.

5.4.4 Natural analogue studies

There have been very few studies of natural analogue evidence for the behaviour of borehole seals in CO_2 storage sites ([186], [190]).

Milodowski et al. [190] describe natural cement clinker and its secondary hydration products at sites in County Antrim, Northern Ireland. The examined natural "cements" occur in contact metamorphic aureoles and skarns around Tertiary dolerite intrusions within chert (flint)–bearing limestone. The analogue clearly differs from the alteration of cement in the presence of supercritical CO_2, but has similarities to the kinds of alteration that might occur if cement should react with CO_2-charged groundwater. Natural CSH gel from the Carneal Plug at Scawt Hill was found to be very similar to the CSH gel in Portland-type cement, and has reacted with CO_2 to form secondary calcium carbonates and silica. Calcite is the dominant secondary calcium carbonate mineral but vaterite and aragonite are also formed. The carbonation was found to have caused the volume of the altered materials to be reduced, with consequent shrinkage and microfracturing of the residual poorly crystalline CSH gel and the silica-rich alteration products. Some secondary calcium carbonate was thought to precipitate in fractures, although these phases were not seen to completely seal the fractures.

5.4.5 Simulations of well seals

A number of studies have attempted to simulate the long-term evolution of well seals in CO_2 storage sites (e.g. [189], [191], [192], [193]). These studies have encompassed both chemical evolution of cements and its coupling with mass transport (e.g. [189], [191], [193]) and thermo-mechanical behaviour of cement (e.g. [192]).

Wilson et al. [189] developed fully coupled models to simulate: (1) a cement carbonation experiment (9 days in duration) reported in [181]; and (2) field observations of cement degradation from the 'SACROC' site (30 years of reaction time) reported in [187]. Although some model input parameters are uncertain, the experimental system was successfully simulated and the model was subsequently 'up-scaled' and applied to the SACROC core data. It was found that as the models were extended to longer time-scales (10^2 – 10^3 years), the effects of parameter and thermodynamic data uncertainties on model output became progressively more significant.

Raoof et al. [193] developed a coupled reactive transport model to simulate the evolution of well bore cement. A Complex Pore Network Model (CPNM) represented the microstructure of the cement by a network of pore spaces and throats. A reactive transport simulator was used to simulate portlandite dissolution and calcite precipitation. Different regions of degradation were identified in the simulation outputs, with increasing distance from the contact between cement and CO_2-charged water: (1) a zone next to the inlet face where dissolution was extensive causing an increase in porosity; (2) a zone of carbonation in which porosity was decreased; (3) the front of carbonation front which had the lowest porosity due to calcium carbonate precipitation; and (4) a dissolution zone.

However, Gherardi et al. [191] drew attention to the pH-buffering capabilities of the wallrocks and cement itself as potentially exerting a significant influence on the evolution of wellbore cement. Their simulations predicted that the cement's matrix would evolve in two stages: an initial "clogging" stage, during which calcite precipitation leads to a porosity decrease; and a subsequent stage of porosity increase, caused by the complete dissolution of primary cement phases, a decrease in calcite precipitation and the re-dissolution of secondary minerals such as Ca-zeolites. As in other studies, the alteration fronts were predicted to penetrate into the cement for only a few centimetres to tens of centimetres over time periods of up to 1,000 years. However, the predicted second phase of porosity increase differed from observations made in experiments (e.g. those of Kutchko et al. [181]) who explained porosity increases as a consequence of calcite redissolution. The difference was explained by the numerical simulations including the buffering of CO_2-rich reservoir porewaters to pH of c. 5 by cement phases.

5.5 Experience from water resources industry

As described in Section 4.5, seals for water resource protection are commonly formed from mixtures of cement and bentonite. The use of such materials is acceptable to the UK regulator and is widely used in the US. We assume that the performance of cement-bentonite mixtures will have been successfully demonstrated through its widespread engineering use. We are not aware of any specific long-term tests to evaluate the performance of cement-bentonite seals after placement.

5.6 Discussion

Chapter 5 presented the approach to understanding the evolution of sealed borehole taken by a number of organisations and industries: RWMOs, oil and gas industry, CO_2 storage industry and water resource industry. We note that extensive RDD has already been carried out on the use of a range of materials to seal and backfill openings in underground repositories. Many of these openings are on the scale of metres or tens of metres, and therefore require large amounts of material to fill them. This is in contrast with borehole sealing, where dimensions are much smaller and the interfacial area with the surrounding rock very high relative to the volume of sealing material. Thus, interactions with the surrounding rocks and groundwater, which might have a small effect on the performance of near-field seals and backfills, might have a much more significant effect on borehole seals.

5.6.1 Seal materials

As noted in Section 4.6.2, selection of materials for borehole seals is strongly influenced by the required longevity of the seal. Natural materials (bentonite, barite and evaporite minerals) are proposed for post-closure seals for boreholes at sites for radioactive waste disposal. In contrast, cement and cement-based materials are widely used for seals in the oil and gas, CO_2 storage and water resources industries. It seems clear that cement-based materials are not generally considered for applications that require very low permeabilities to be maintained for timescales greater than many thousands of years. The exception is the use of salt-saturated cements for some post-closure seals in evaporites; note that long-term creep of evaporite rocks around a borehole is expected to contribute to sealing in this environment.

The approach to demonstrating longevity of natural materials in geological systems is generally based on geological observations with supporting interpretative modelling. Bentonite has been extensively studied in a range of groundwater environments; both to determine the impact on the swelling capacity of bentonite and on any mineralogical changes to the bentonite. Investigations in freshwater, seawater environments and brines confirm the stability of bentonites over geological timescales.

Illitisation of montmorillonite has been studied extensively in the oil industry, especially in relation to the role it plays in creating and maintaining formation over-pressures in shales, thereby affecting drilling operations, and also of the impact of this diagenesis and mixed-layering on reservoir quality. Studies have also been undertaken by RWMOs. These oil industry and geological waste disposal studies indicate that not only is a significant flux of dissolved potassium necessary for illitisation of montmorillonite, but also that temperatures higher than those likely to be encountered by a borehole seal are required to cause extensive illitisation.

CO_2 storage experience provides some qualitative support for the longevity of Portland cement-based seals on timescales of at least thousands of years under in-situ conditions that are likely to be chemically more aggressive than those occurring in site characterisation boreholes drilled in order to develop a GDF. However, many of the outstanding uncertainties that apply to seals in such GDF-related site characterisation boreholes also apply to CO_2 storage; the length of time for which seals must maintain adequate performance is much longer than the duration of any laboratory or field experiments. Experience from the CO_2 storage sector also highlights the importance of permeable pathways within sealing materials. Provided that there are no permeable pathways such as fractures, reactive CO_2-charged waters cannot gain access to the bulk of the cement, which therefore retains its sealing properties. The coupling between the development of fluid flow pathways and reactions between formation fluids and cement is therefore critical. The development of flow pathways could be a predominantly mechanical phenomenon, depending upon the stress state of the borehole walls.

The oil and gas industry considers that natural movements of the formation around the borehole contribute to the effectiveness of the seal over longer times. Similar arguments are deployed by RWMOs. The potential reversibility of an Excavation Damage Zone (EDZ) created around repository openings is discussed in Section 5.2 of [5], where it states '*over long time periods, the effects of an EDZ in evaporites and lower strength sedimentary rocks are expected to have largely disappeared. In contrast, an EDZ in higher strength rocks may be a long-lived feature.*' Whilst reversibility of an EDZ around large openings in LSSR are considered, this has not yet been taken into account when considering evolution of borehole seals in such materials.

5.6.2 Plug/backfill materials

These materials will be exposed to higher fluxes of groundwater and to higher groundwater velocities than the seals. Higher groundwater velocities are an issue for bentonite-based materials, as erosion or piping of such materials by flowing water can occur under some conditions. Erosion of bentonite may be of concern if it is used for plug/backfill materials, because these materials are required to provide long-term mechanical support to any overlying seals. In Section 4.2.2.5, we note the potential for using sand-bentonite mixtures, which might reduce the potential for bentonite erosion.

Cement and cement-based materials are widely used (e.g. by the oil and gas and water resources industries) and proposed (e.g. by RWMOs and the CO_2 storage industry) for the components that are located between the seals. See Section 4.6.3. Cement minerals will not be in equilibrium with the surrounding rocks, and extensive experimental and modelling studies have demonstrated this. Natural analogue evidence is that CSH phases can persist in groundwater over timescales of tens of thousands of years, possibly because reaction products tend to seal the system and protect the CSH from further reaction. The durability and condition of Roman pozzolanic cements after 2,000 years immersion in seawater is such that researchers conclude it is difficult to assess if immersion in seawater has had a deleterious effect.

5.6.3 Interactions between seal components

Chemical reactions between different components used to seal boreholes will occur if they are not chemically compatible. These interactions are unlikely to result in significant changes to seal properties over timescales of tens of years; if they did, such combinations of materials would not be acceptable. However, longer-term sealing performance might be compromised.

The principal interaction considered is that between bentonite and cement. Laboratory experiments and modelling confirm that mineralogical charges will occur, with subsequent changes to the bentonite swelling pressure, porosity and other characteristics. Natural analogues confirm mineralogical and physical property changes, but also demonstrate the limited spatial extent (in the order of millimetres or centimetres) of these reactions in the systems studied. This is also consistent with model results, and may be the result of the tendency of reaction products to seal porosity and reduce groundwater flow. See Section 6.3 for illustrative geochemical calculations that highlight some of these issues. The results of the analogue studies suggest that the reaction zone between a cement component and a bentonite component in a borehole might be limited. If the bentonite and cement were mixed in a single material, reactions and consequent changes might be more extensive.

5.6.4 Testing and validation of borehole seals

The oil and gas industry only deploys seal materials after a sequence of development, qualification, installation and verification. Extensive laboratory materials testing is undertaken to determine permeability, stability to fluids, dimensional stability and mechanical strength. Extensive QC takes place at the wellhead prior to placement of materials. Once placed, there is no practicable potential for recovering seal materials for testing. Thus, testing of seals is generally restricted to downhole permeability testing to establish the overall integrity of the seal.

6 Additional calculations to support development of a programme of generic RDD into borehole sealing

6.1 Introduction

RWMD's Scope of Work for this project [8] requires that additional numerical analysis is undertaken to advance '*RWMD's knowledge on borehole sealing and the requirements to be met by the engineering process pursued, and the materials utilised, to seal site investigation boreholes in a UK context*'.

This Chapter presents a summary of the calculations undertaken as part of the project. The objective of these illustrative calculations is to identify key issues relevant to borehole sealing. The output from the calculations is used to inform our recommendations for a programme of generic RDD into borehole sealing (see Chapter 8). Further information on the calculations is presented in Appendix 1 and Appendix 2.

Section 6.2 presents the results of simple 1D analytical calculations of groundwater flow in and surrounding a sealed borehole. The objective is to demonstrate, for the range of parameter values presented in Chapter 3, where the principal resistances to flow might occur. The required permeability of a borehole seal relative to the permeability of the surrounding rocks and the BDZ is informed by these calculations.

Section 6.3 presents the results of geochemical calculations that consider the chemical, mineralogical and volume changes that occur in bentonite seals as a result of interaction with surrounding groundwaters (compositions taken from Chapter 3) and with cement, which may form part of the support elements in the sealed borehole. These calculations illustrate how important these changes might be and, in particular, estimate the spatial scale over which alteration of the bentonite seal might be expected. Uncertainties introduced by modelling highly saline solutions are also illustrated.

6.2 Additional groundwater flow calculations

In this Section, the effects of open and sealed boreholes on groundwater flow in the vicinity of a Geological Disposal Facility (GDF) are discussed. The analytical model presented in the following Sections is simple, and comprises three flow resistances arranged in series:

- flow to the borehole through a transmissive feature in the surrounding rock;
- flow along the borehole;
- flow away from the borehole through a transmissive feature in the surrounding rock.

Flow along the borehole is itself represented as four flow resistances arranged in parallel, to represent flow through the seal, at the interface between seal and surrounding rock, within the Borehole Disturbed Zone (BDZ) and in the surrounding undisturbed rock. A description of the system is given in Section 6.2.1. A description of the analytical model is given in Appendix 1. Calculations from the model are presented in Section 6.2.3.

6.2.1 Description of the system

An open borehole provides effectively negligible resistance to water flow along the borehole. If an open borehole connects two or more transmissive features[1], it will form a transmissive connection between them. See Figure 6-1, in which groundwater flows to the borehole in one feature and away from the borehole in the other feature. Such flows would occur if the 'undisturbed' groundwater heads in the features are different, which would usually be the case.

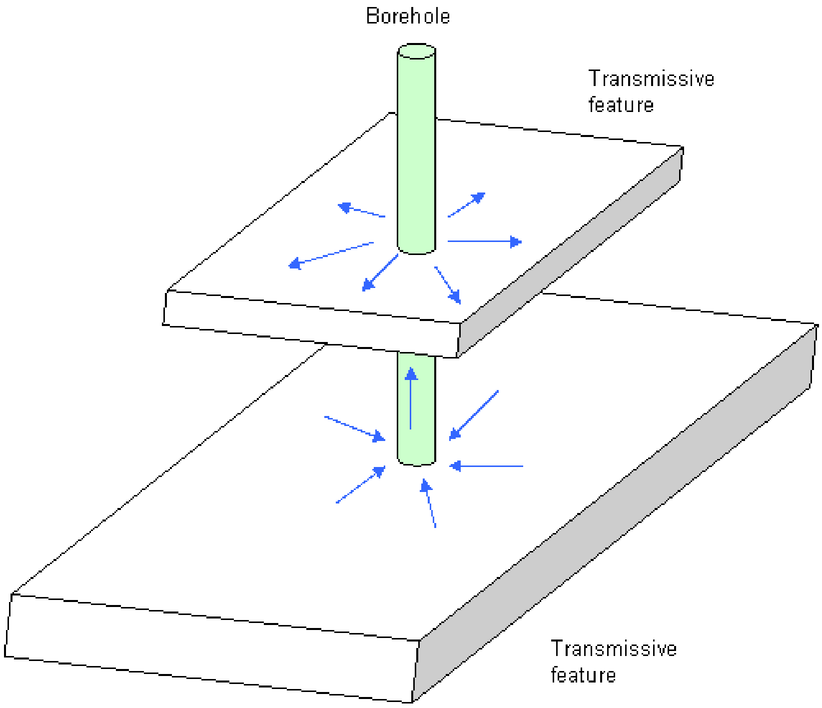

Figure 6-1 Flows as a result of a borehole linking two transmissive features

The flows resulting from the presence of the open borehole (or boreholes) could modify the pathway for migration of radionuclides from a GDF and even lead to new pathways. The significance of the modifications to the groundwater flow in the vicinity of a GDF and the modifications to radionuclide pathways for the performance of the GDF resulting from the presence of open boreholes would be specific to the site in question. At some sites, the effects resulting from the presence of the open boreholes might be negligible, whereas they might be important at other sites.

In order to mitigate or prevent the effects illustrated in Figure 6-1, it is envisaged that boreholes would be sealed once any measurements to be made in the boreholes have been completed. The seals may degrade over the very long times that need to be considered in assessing the performance of a GDF (of order a million years). Some simple models for the potential effects of seals and some illustrative calculations are presented below.

1 A transmissive feature might be a transmissive fracture, a transmissive fracture zone or a very permeable rock formation

Simple models are presented In Appendix 1 for flow to/from a borehole in a transmissive feature and for flow along a section of borehole between intersections with transmissive features. As indicated by the discussion in Appendix 1, there may be a number of different sealing components between the intersections. These different components will have different properties and might degrade differently over time.

For each section of sealed borehole, three potential paths for flow can be identified (see Figure 6-2):

- Flow along a degraded seal
- Flow along the boundary between the seal and the surrounding rock
- Flow in a possible damaged zone of rock immediately surrounding the borehole

In addition, we consider flow through the undisturbed rock surrounding the borehole.

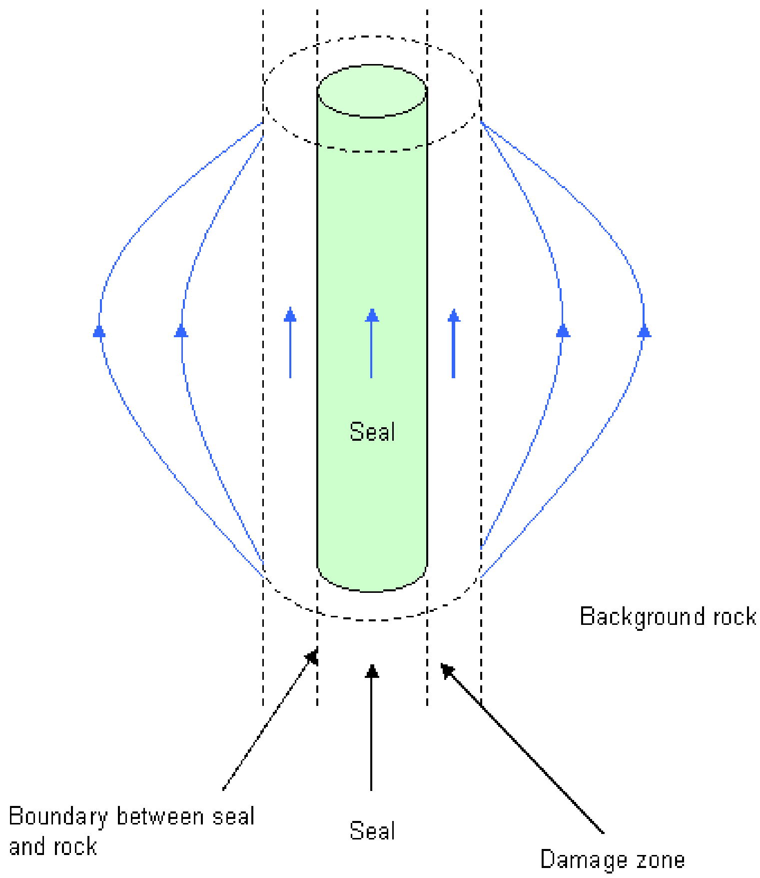

Figure 6-2 Flow paths for a section of sealed borehole

At first sight, it might seem odd to include the last path, and indeed, it would not be appropriate to treat flow through the undisturbed rock along the whole length of the borehole as flow along the borehole. However, as discussed above, it is possible that some sections of sealed borehole will have significant flow along the seal, the boundary between the seal and the surrounding rock or the damaged zone. These may be separated by sections where the seal has not degraded significantly, and there is little flow along the seal, the boundary between the seal and the surrounding rock or the damaged zone (see Figure 6-3). In such cases, the flow along the borehole may be controlled by the flow through the undisturbed rock in those sections where the seal has not degraded significantly.

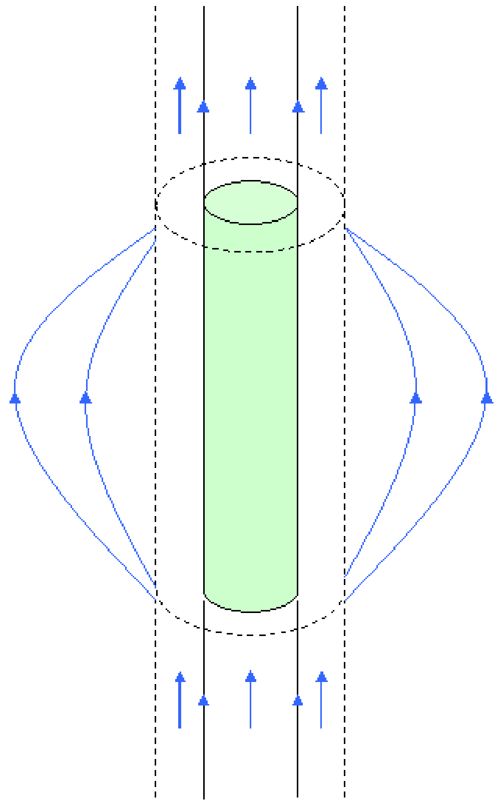

Figure 6-3 Flow through the background rock linking two flowing sections of borehole

Simple steady-state models can readily be developed for each of the first three flow paths: see Appendices 1.2.1 – 1.2.3. A model for the last flow path can also be developed as discussed in Appendix 1.2.4.

6.2.2 Calculations of flow resistance

A specific site for a GDF has not been chosen in the UK, so the geological sequence that boreholes might pass through is not known and the properties of the different rocks are not known. Further, no attempt has been made in this section to quantify the properties of degraded seals or the time scales for degradation. Rather, some illustrative values of the various flow resistances are presented, based on parameter ranges presented earlier in this report. The aim is to illustrate the dependence of the flow resistances on key parameters.

The overall flow resistance corresponding to particular combinations of the different resistances can readily be obtained by combining appropriately the different resistances. In most cases, it is sufficient simply to identify the controlling flow resistance. Calculated flow resistances are presented in Appendix 1.4.

6.2.3 Illustrative calculations

Illustrative values of hydraulic resistances are presented in this Section. Hydraulic conductivities from which some these resistances are calculated are based on ranges presented in Table 3-1.

For the parameter ranges considered in Table A1-1 to Table A1-5, the flow resistance of a transmissive feature greater than >10^{-7} m^2s^{-1} is always lower than that of the undisturbed rock, the borehole disturbed zone and the interface between seal and rock. For these parameter values, flows to and way from the borehole are never limiting. This is as expected; we do not consider flows in transmissive zones further.

The tables below illustrate some relevant hydraulic resistances (defined as above) for different pathways and different parameter values.

Table 6-1 Illustration of flow resistances for different components of the system

Pathway	Parameter	Parameter value	Flow resistance (s m^{-2})
Flow to/from borehole in transmissive feature	Transmissivity	10^{-5} m^2s^{-1}. Upper bound for major fracture zones in HSR	1.1 E+05
		10^{-8} m^2s^{-1}. Lower bound for major fracture zones in HSR	1.1 E+08
		10^{-10} m^2s^{-1}. Typical fracture transmissivity in HSR away from major fracture zones	1.1 E+10
Undisturbed rock	Hydraulic conductivity	10^{-13} ms^{-1}. Lower bound for HSR and LSSR	1.6 E+12
		10^{-10} ms^{-1}. Upper bound for LSSR	1.6 E+09
		10^{-9} ms^{-1}. Upper bound for HSR	1.6 E+08
Borehole Damaged Zone	Hydraulic conductivity (assumed to be 10 times that of undisturbed rock). Thickness of BDZ equals borehole radius	10^{-12} ms^{-1}. Lower bound for HSR and LSSR	8.5 E+15
		10^{-9} ms^{-1}. Upper bound for LSSR	8.5 E+12
		10^{-8} ms^{-1}. Upper bound for HSR	8.5 E+11
Interface between seal and rock	Equivalent hydraulic aperture	1,000 µm (equivalent to 5% shrinkage of seal volume[a])	7.6 E+06
		30 µm (equivalent to 1% shrinkage of seal volume[a])	2.6 E+10
Through seal	Hydraulic conductivity	10^{-13} ms^{-1}. Equal to lower bound hydraulic conductivity for HSR and LSSR	2.6 E+17
		10^{-10} ms^{-1}. Equal to upper bound hydraulic conductivity for LSSR	2.6 E+14
		10^{-9} ms^{-1}. Equal to upper bound hydraulic conductivity for HSR	2.6 E+13

Notes

[a] The equivalent hydraulic aperture is calculated on the assumption that all shrinkage is expressed by the formation of a uniform aperture void between borehole wall and seal

For the parameter ranges considered, the main points from Table 6-1 are:

- resistances associated with flows into and out of the sealed borehole from the surrounding rocks are generally much smaller than resistances associated with flows along the borehole. That is, for the parameter ranges considered, flows through the sealed borehole are controlled by whichever of the seal, interface, BDZ or surrounding undisturbed rock has the lowest flow resistance. It is, of course, the case that if the transmissivity of the rocks above and below the seal is sufficiently low, flow through the rock will become the limiting factor. This should be explored in future modelling.
- comparison of the various flow resistances along the borehole show the following:
  - for the case where hydraulic conductivity of the seal and undisturbed rock are equal, the scoping calculations indicate that flow is overwhelmingly through the undisturbed rock. The flow resistance of the seal is nearly five orders of magnitude greater than that of the undisturbed rock around the borehole;
  - notwithstanding the enhanced hydraulic conductivity of the BDZ relative to the undisturbed rock, flow is predominantly though the undisturbed rock for the representation of BDZ chosen. The flow resistance of the BDZ is approximately 5,000 times greater than that of the undisturbed rock around the borehole;
  - shrinkage of the seal and generation of cracks at the interface with the rock has the potential to generate flows that are significantly greater than through either the seal or the BDZ. Shrinkage of the seal volume by 1% potentially generates a flow at the interface equivalent to that through a seal with hydraulic conductivity of 10^{-6} ms^{-1}.

The scoping calculations emphasise the importance of (i) understanding the standard of sealing required and (ii) the generation of cracks in the seal, for example those formed by shrinkage due to mineral reactions.

6.3 Additional geochemical calculations

6.3.1 Rationale and approach for geochemical calculations

This Section presents the results of chemical calculations that are intended to illustrate some key issues, thereby highlighting topics for further investigation. Full details of the calculations are given in Appendix 2.

Simulations of the behaviour of bentonite and cementitious components of a borehole sealing system are inevitably complex and must represent many variables (including solid phase and water compositions, transport parameters, temperature, geometries etc). Furthermore, for practical reasons simplifications must be made when representing a particular conceptual model of a seal system using a given numerical model. Choices must also be made when selecting thermodynamic and kinetic data and the underlying numerical models (e.g. activity models and rate equations). It must be recognized, too, that inevitably any given database of thermodynamic or kinetic data will have associated inaccuracies and uncertainties. To investigate the potential significance of all these factors for our understanding of borehole seal performance in the long-term would require a substantial programme of work. The present project has not attempted to undertake such an investigation. The approach taken was to:

- carry out a limited number of new calculations using Quintessa's CABARET software; and

- additionally to review outputs from previous simulations undertaken by Quintessa to investigate the behaviour of cementitious and bentonite-bearing barrier materials, in the light of the requirements for the present project.

The new simulations used Quintessa's CABARET (Cement And Bentonite Alteration due to REactive Transport) software, v1.0.2. The current version of CABARET is able to simulate reactions between cementitious materials and bentonite in multiple dimensions. CABARET allows users to specify cement-bentonite-rock-water systems flexibly, in terms of the chemical components present, the physical geometry of the simulated system and the processes to be represented. Chemical and transport processes can be fully coupled to one another so that, for example, porosity changes due to mineral precipitation and dissolution are coupled directly to the transport and flow processes. The software can import thermodynamic databases in Geochemist's Workbench™ [194] format, allowing a wide range of industry-standard databases to be used without modification.

The new simulations, for both bentonite-based seals (Section 6.3.2) and cement-based seals represented a section of borehole, as shown in Figure 6-4.

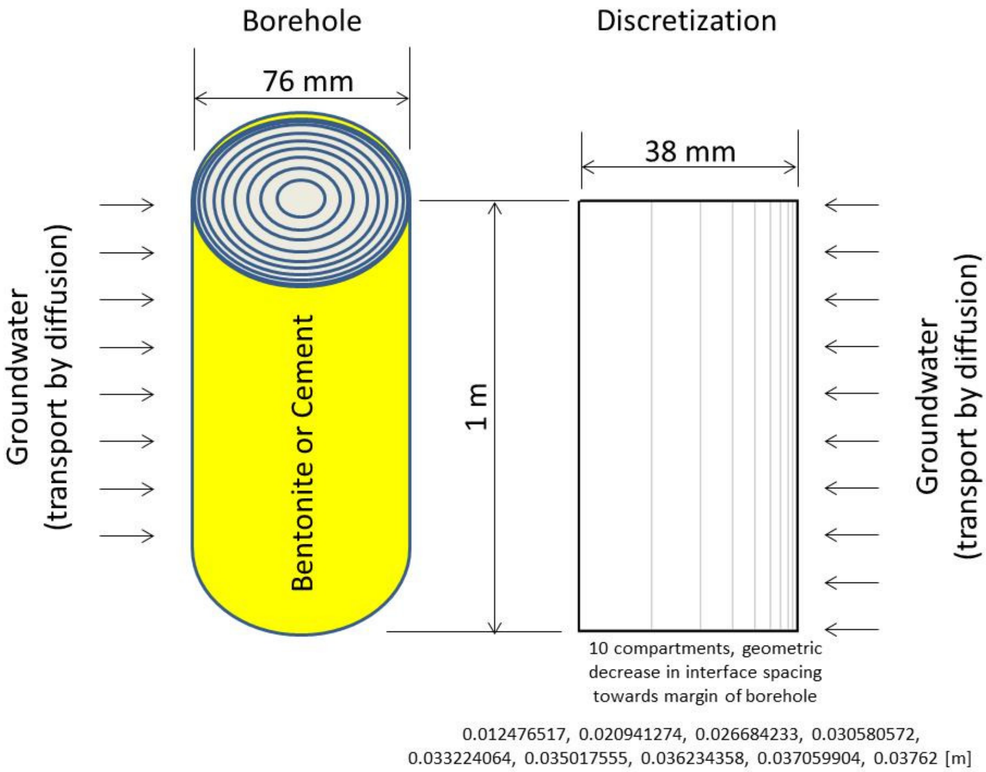

Figure 6-4 Schematic representation of a borehole section in the CABARET simulation

The model borehole has a diameter of 76 mm, which is approximately half that of the smallest borehole currently being considered by RWMD. See Section 2.2.2. This diameter was chosen for the models because it would result in a greater proportion of seal alteration than would occur in a larger diameter borehole; seal alteration would be maximal in the models.

The numerical models, data and key results are described in detail in Appendix 2. A summary is given in Sections 6.3.2 to 6.3.5. Conclusions from the illustrative calculations are presented in Section 6.3.6.

6.3.2 Bentonite-based seals

The calculations (Figure A2-2, Figure A2-3), which consider the interaction of bentonite with a range of illustrative groundwater compositions, showed that the bentonite approaches cation exchange equilibrium across the entire width of the seal after about 50 years. Depending on the nature of the ion exchange with the groundwater there would be a reduction in swelling pressure, although this is likely to be small in this case for the dry densities of relevance to borehole seals (e.g. [195]). The timescale for alteration is a minimum, for two reasons:

- firstly, these simplified simulations specified a fixed water composition at the borehole wall. In reality, these seals would be emplaced in low-permeability rocks where mass transport through the rock would likely be dominated by diffusion. In these circumstances, diffusive fluxes through the rock will not be sufficiently high to maintain constant groundwater compositions at the borehole wall. Consequently, the rate of alteration of the seal would reduce over time;
- second, the simulated borehole diameter is at least a factor of two smaller than borehole diameters currently being considered by RWMD. Simple models would suggest that the timescale for ion exchange to be completed would be proportional to the diameter squared. Hence, this effect might increase the timescale by at least a factor of four.

For simulations with both fresh and saline water compositions, the porosity of the bentonite was calculated to decrease over time in the vicinity of the outer surface of the seal (Figure A2-4). The principal cause of the porosity loss near the outer margin of the bentonite was the precipitation of saponite, an Mg-rich smectite clay.

6.3.3 Cement-based supports

Illustrative simulations were also undertaken for cementitious (C1) support elements. The basic geometry employed in the simulations was as shown in Figure 6-4. The cement composition was a simplified representation of a Class G cement, which is commonly used in borehole sealing. Cement-based supports would be employed where a borehole intersects relatively permeable rock. In these circumstances, transport of solutes to the borehole wall is likely to be dominantly by advection. Therefore, the fixed water chemistry at the borehole wall specified in the model is likely to be more representative of the real situation than in the case of the bentonite seal described in Section 6.3.2.

For simulations using both fresh water and saline water, the proportion of tobermorite increased relative to jennite towards the margin of the support (Figure A2-7) reflecting the progressive preferential leaching of Ca from the cement at a faster rate than leaching of Si. These reactions are accompanied by a porosity reduction near the margin (Figure A2-8). The porosity reduction at the boundary in both cases was caused by precipitation of calcite (Figure A2-9). In addition, in the saline water case, ettringite also precipitated in a significant quantity, leading to further porosity reduction (Figure A2-9).

6.3.4 Cement-bentonite interactions

In the present work cement-bentonite interactions were not investigated by means of new calculations. However, a previous CABARET test case had been constructed to investigate further the cement-bentonite models described by [196]. In these models, a cementitious porefluid of fixed composition is specified to occur at the margin of a bentonite. These changes are illustrated for a simulation of 1000 years duration in Figure A2-10. We conclude that the net consequence is that overall the alteration caused by cement-bentonite interactions extends no more than a few tens of centimetres into the bentonite.

6.3.5 Uncertainties regarding salinity

All the simulations reported here have considered only fresh and saline groundwater (Table 3-3, Table A2-2). However, in much of the UK deep groundwaters are brines, which are much more saline than the considered saline groundwater. 'Conventional' geochemical models are inappropriate for simulating reactions involving such brines because the models that they use for activity coefficients (commonly either the Davies model or the Debye-Hückel model) become increasingly inaccurate for salinities greater than that of seawater. Instead an alternative approach is needed to calculate activity coefficients in brines. The potential significance of the limited ability to simulate reactions in the presence of highly saline groundwaters is illustrated by some scoping calculations that are reported in [197].

It can be seen (Figure A2-11) that simulations employing both the Davies approach and the Pitzer approach give broadly similar results over short timescales of 30 years. After this time, the results diverge. In particular the choice of the Davies model leads to a thicker alteration zone in this model. One implication of these results is that even if models are successful at reproducing short-term observations, for example those obtained from laboratory experiments or field investigations of operating wells, they may not necessarily be reliable in the long term.

6.3.6 Conclusions from illustrative geochemical calculations

The simple illustrative simulations presented here do not explore all aspects of the long-term behaviour of bentonite and cementitious components of a borehole sealing system. However, they do illustrate the potential significance of a number of processes and indicate minimum timescales over which high proportions of a seal may alter. The simulations show that certain processes that have been shown to be unimportant influences on the performance of the bentonite buffer systems around waste canisters, may be much more important given the different geometry of a borehole.

Diffusion alone can plausibly cause all the bentonite within a seal to reach cation exchange equilibrium with the surrounding groundwater relatively rapidly, provided that the transport properties of the rock (which were not investigated) do not limit the supply of solutes to the seal or support element. This process can occur because diffusion from the margin of the seal to the centre can occur over a timescale shorter than that required for porosity reduction in the marginal zone to slow mass transport into the seal. In previously studied geometries such as buffers surrounding waste canisters, where the bentonite has a much larger mass for a given surface area in contact with the surrounding groundwater, the entire volume of bentonite may not exchange cations before the porosity reduction slows the rate of mass transfer.

The overall significance of cation exchange for bentonite seal performance is unclear. Most likely there will not be a significant impact upon swelling pressure for the relevant dry densities in the presence of most fresh and saline groundwaters that are likely to be encountered in the UK (c.f. [195]). However, most studies of bentonite properties in repository environments have focussed on dominantly Na-exchanged bentonite, and less work has been carried out on bentonites with other cation populations (e.g. Ca-exchanged bentonite), so that there remain some uncertainties regarding the overall effect of cation exchange on performance (e.g. [198]).

Similarly, the simulations illustrate that the water composition will have an important effect on the long-term evolution of cementitious supporting elements. In the presence of fresh groundwater diffusion alone could drive an increase in porosity throughout the diameter of the borehole in only a few tens of years. In contrast, in saline groundwater porosity decreases due to water-cement interactions could potentially slow the rate of mass transport to the extent that the majority of the cementitious support element remains little altered. The overall impact of these processes on the effectiveness of a sealing system is presently unclear.

Reactions between cementitious support elements and adjacent bentonite seals are unlikely to lead to alteration of the bentonite over distances of more than a few tens of centimetres. If the length of the bentonite seal is long compared with this zone (which is almost certain to be the case) then the overall effect on the performance of the seal will be small. Furthermore, on the basis of these calculations, the distance over which the bentonite's performance will be impaired is likely to coincide with the zone of enhanced porosity, which is significantly shorter than the overall distance over which reactions occur. However, it should be noted that these calculations did not consider the effect of the alteration on the mechanical properties of the sealing materials. It is possible that these effects could be detrimental to seal performance, for example if the porosity reduction also makes the seal more brittle and hence more susceptible to fracturing.

Alteration of the kind simulated here would potentially be more significant where a bentonite seal is emplaced adjacent to cement that occurs in the borehole walls. Such cement may have originally formed a bond behind a casing that has since been removed, or alternatively could be grout that has been used to seal fractures. In such cases, a more significant proportion of the bentonite might potentially alter.

The available thermodynamic and kinetic data limit our ability to predict confidently the future evolution of bentonite seals and cementitious sealing elements. All the simulations predicted that saponite would replace montmorillonite near the margin of bentonite seals. However, while saponite does occur in natural bentonite deposits, such pervasive replacement of montmorillonite is not typically observed. This discrepancy implies that the available kinetic data and / or thermodynamic data may not allow accurate simulations of real-world alteration processes.

A more significant limitation is our ability to simulate accurately the evolution of bentonite seals and cementitious support elements in the presence of very saline groundwaters, which are widespread in the UK. 'Conventional' approaches for calculating the activity coefficients of aqueous species are inapplicable in such circumstances. Approaches such as the 'Pitzer approach', which are applicable to brines, are limited in their application by a lack of appropriate thermodynamic data.

The calculations did not investigate the coupling between chemical processes and the evolution of mechanical properties. Leaching of cement from a cementitious support element would presumably result in a decrease in its mechanical strength. Similarly, the reduction in porosity that accompanies mineralogical alteration of bentonite near the interface with cementitious material could potentially lead to an enhanced likelihood of cracks developing. It would be valuable to investigate this coupling between chemical processes and mechanical properties in order to establish whether it could influence the overall performance of a borehole sealing system.

7 Functional requirements for components of RWMD's borehole sealing systems

7.1 Introduction

RWMD site investigation boreholes are to be sealed using a combination of 'seals' and 'support' elements. In RWMD's Sealing Objective 2, a clear distinction is drawn between sealing for protection of water resources (water resource seals) and sealing to ensure that the borehole does not have a significant adverse impact on the long-term environmental safety case for a GDF (post-closure seals).

Post-closure seals have a sealing function on timescales as required by post-closure performance assessment. In the context of deep site investigation boreholes for a GDF, only some sections of borehole will require sealing from a post-closure performance perspective. Such post-closure seals will be placed within the host rock and at key locations in overlying cover rocks. The prime purpose of 'supports' is to provide mechanical support to post-closure seals on these same timescales. Protection of groundwater might be required at some of these locations. Thus, even if a section of site investigation borehole does not require sealing for post-closure purposes, it will still be necessary to meet the requirements of water resource protection.

In the following sections, we recommend functional requirements for post-closure seals and supports, both at placement and in the long-term. First, in Sections 7.2 and 7.3, we consider the overall issues around requirements for permeability and longevity. These considerations are informed by RWMD's sealing objectives, the reviews in Chapters 4 and 5, and the illustrative calculations in Chapter 6.

7.2 Consideration of permeability requirements

The following considerations apply to post-closure seals:

- the standard of sealing required against groundwater flow and gas migration will be informed by the requirements of post-closure performance. As the way in which post-closure safety can be achieved will be influenced by the nature of the geological setting, quantitative requirements on seals cannot be fully defined yet. Nevertheless, understanding the potential range of seal permeabilities required in different geological environments and disposal concepts will be an important early component of the generic phase of RDD, in order to assess the appropriateness of various seal concepts;
- at the generic stage of the sealing programme, we wish to understand the potential permeability that can be achieved by different seal concepts in the range of geological conditions potentially relevant to a UK GDF. For comparison, Chapter 3 presents indicative permeability ranges for these geological settings. We recognise that the performance required will be optimised during the subsequent site-specific phase of RDD;
- radionuclide transport in rocks with very low permeability will be diffusion-dominated. In cases where such rock is to be sealed (for example, LSSR and unfractured sections of HSR), it is unlikely that the seal permeability will need to be as low as that of the host rock. (Transport of radionuclides into the borehole will be by diffusion, not

advection.) We suggest that calculations should be undertaken in the generic RDD programme to explore the standard of sealing likely to be required in a rock where radionuclide transport is diffusion-controlled.

With regard to water resource protection, the requirement in Environment Agency guidance [13] is either to mimic the permeability of the surrounding rocks and soils or to place a low permeability backfill throughout the borehole.

7.3 Consideration of longevity requirements

Two principal aspects need to be considered: permeability and mechanical stability. The evolution of properties over timescales of relevance will also need to be understood, unless arguments can be made that there is no change in properties with time.

If long-lived low permeability is required on timescales of relevance to post-closure safety, which may be up to several million years [5], then it will be necessary to use natural materials that do not undergo significant detrimental interactions (in terms of permeability change) with the environment in which they are placed. Use of engineering-based materials such as cements can achieve low permeability at the time of placement and on the scale of hundreds of years thereafter, but it is unlikely that a robust argument could be made that low permeability persists for more than several thousands of years, in particular in the case of borehole seals where the horizontal dimensions of the placed material are so small. Longevity of seals and backfill is not discussed in EA guidance for water resource protection [13], but the implication of the guidance is that sealing is required on timescales of order hundreds of years.

We propose the following to enable a generic RD&D programme to be appropriately focused:

- the B1, B3 and CC-S illustrative seal concepts presented in Section 2.5 are all post-closure seals. They will require a longevity on a timescale as required by the Environmental Safety Case;
- the B2 and C1 illustrative seal concepts presented in Section 2.5 are both support elements. These, and any remaining backfilled sections of cased borehole, will need to provide mechanical support for the timescales required by the post-closure seal elements. They will also need to meet the sealing and backfilling requirements for water resource protection, which require low permeabilities on timescales achievable by cement-based materials. Some support components may require a specific low permeability at placement to enable adjacent seals to be installed.

Lastly, interactions between adjacent seal or support components in the borehole must be considered. Here, the main issue is the potential effect of any cement-based component on adjacent clay-based components. If cement-based components are used, it will be necessary to demonstrate that the magnitude of any changes or the proportion of the clay-based component affected is sufficiently small that the longevity and performance of the clay-based seal are not compromised. Such demonstration can be based on and benefit from work performed to date for repository seals.

7.4 Suggested functionality of post-closure seals

Post-closure seals for HSR, LSSR and evaporites are all required to provide a long-term seal against key low permeability sections in the host rocks. The standard of sealing required against groundwater flow and gas migration will be informed by the requirements of post-closure performance. Post-closure seals provide this seal for as long as is required by the post-closure Environmental Safety Case. Previous RWMD post-closure assessments have been performed to a timescale of 1 Ma, so potentially some sealing performance to this timescale may be required. Where the full casing string has been locally or completely removed from cover rocks, the post-closure seals are also required to seal against key low permeability sections in the cover rocks. The longevity of these post-closure seals can only be achieved in HSR and LSSR through the use of natural materials that are stable in contact with the surrounding rock. In the case of evaporites, where closure of the borehole due to long-term creep of the surrounding rocks is likely to contribute to long-term sealing, it is possible that post-closure seals could be formed from either natural or engineered materials.

The permeability required of post-closure seals will be informed by the requirements of post-closure performance, rather than to return the rock to its pre-drilled condition. A consequence of this approach might be that the permeability required for a post-closure seal located in the host rock may be higher than that required for a post-closure seal located in overlying cover rocks.

For information, Table 3-1 presents illustrative permeabilities of generic host rocks and possible cover rocks relevant to the UK geological disposal programme.

- The hydraulic conductivity of LSSR host rocks is estimated in the range 10^{-10} ms^{-1} to 10^{-13} ms^{-1}; that of HSR over length scales of tens of metres (the potential length scale of seals) is in the range 10^{-9} to 10^{-13} ms^{-1}. For comparison, the permeability of the SKB reference design (which forms the basis for RWMD's illustrative B1 seal concept) has been measured and calculated to be 10^{-12} ms^{-1}, although the required performance in the context of the Safety Case (SR-Site) could be met with a seal permeability that is three to four orders of magnitude higher. In the case of SKB, the requirement is for this seal to have a life of at least 100,000 years.
- For evaporite host rocks, a range from 10^{-10} to 10^{-14} ms^{-1} is suggested for halite (higher values correspond to strained salt); in anhydrite, permeability is considered to be higher (10^{-8} to 10^{-13} ms^{-1}). Potentially, inter-beds with higher permeabilities would require sealing if evaporites were encountered in cover rocks.

The RWMD illustrative borehole concepts recognise that some casing may be left in-situ (see Section 2.2.3). This is most likely to occur in cover rocks, but it could also occur in HSR and LSSR host rocks. Depending on the site, it may be necessary to install post-closure seals in these one or more of these sections of borehole. The function of these post-closure seals is to limit long-term groundwater flow in the annulus between casing and borehole wall, after the cement bond has degraded. To effect a post-closure seal, it will first be necessary to locally remove the casing to enable the seal to directly contact the rock. See Section 2.2.3. The functional requirements of a post-closure seal installed where casing has been locally removed will be the same as for a post-closure seal installed in areas where casing has been fully removed.

7.5 Suggested functionality of support elements

We propose that the post-closure role of support elements is to provide mechanical support for any overlying post-closure seals in the borehole. Support elements must therefore provide suitable mechanical support for the lifetime of the seals; as described in Section 7.4, this may potentially be up to of order a million years.

In addition, support elements in some locations will be required to provide water resource protection, most probably over a timescale of hundreds of years. See Section 4.5.1 and [13], where it is suggested that cement-based materials would have permeabilities suitable for such a purpose (note: we are not suggesting such materials would be suitable; only that materials which achieved such permeability in the short term would probably be acceptable to EA). Our view is that support components are not required to provide water resource protection in the longer term.

Table 3-1 presents illustrative hydrogeological properties for a range of sedimentary cover rocks. They range from highly fractured limestones with permeabilities as high as 10^{-2} ms^{-1}, through to permeable clastic rocks (hydraulic conductivities typically in the range 10^{-8} to 10^{-5} ms^{-1}) and lower permeability finer-grained rocks (hydraulic conductivities typically in the range 10^{-10} to 10^{-13} ms^{-1}). EA's requirement is that boreholes are abandoned either by placing materials that mimic the permeability of the surrounding rock or which are of low permeability. The implication is that a range of designs, and materials, will be required for support elements. For the purposes of a generic RDD programme, we suggest that two types of sealing elements are required:

- support element for higher permeability sections (for which the RWMD illustrative seal concept is C1);
- support element for lower permeability sections (for which the RWMD illustrative seal concept is B2).

The potential for seals to be damaged during placement because of inflows or outflows from adjacent transmissive zones is recognised. In order to protect seals from such flows, support element for higher permeability sections may be required to have a low permeability at the time when adjacent seals are placed. Beyond this potential short-term requirement, they have no sealing function.

A range of materials is potentially suitable for support elements: for example, cement, bentonite and crushed rock. Given the suggested functional requirements, we do not rule out use of any of these materials at this stage.

8 Key issues for RWMD's future programme of generic RDD into sealing deep site investigation boreholes

8.1 Objectives of the generic RDD programme

The output from the generic RDD programme into sealing deep site investigation boreholes must be sufficient and suitable to meet EA's requirements regarding borehole sealing (see Section 1.1), in order to enable EA to issue an Environmental Permit for intrusive investigations in a timely manner. To enable this, the generic RDD programme into sealing deep (i.e. >200m) site investigation boreholes needs to demonstrate that RWMD has developed generic approaches to sealing boreholes, and is confident that site investigation boreholes can be successfully sealed against groundwater flow and gas migration in the range of geological settings potentially relevant for a UK GDF. As noted in Section 2.5.1, conceptual designs for seals and supports at the time of the ISE submission might not be fully optimised. They may provide a higher degree of sealing than is required. Once an intrusive surface-based site investigation is underway, RWMD will use the outcome from the generic RDD programme as the basis of understanding from which to develop a programme of site-specific RDD on borehole sealing.

RWMD's B1, B2, B3, C1 and C-SS illustrative seal concepts are based on the view of participants at an RWMD workshop [11] that these concepts can probably be successfully applied to the range of geological settings and borehole designs potentially relevant to RWMD. We recommend that all these illustrative seal concepts be considered in the generic RDD programme.

RWMD has defined the current report as the deliverable from 'Phase 1' of research into sealing deep site investigation boreholes. The current report contains recommendations for a generic RDD programme into borehole sealing. Strictly, this phase of the project will be 'Phase 2'. However for simplicity we refer to this future programme simply as the 'generic RDD programme'.

Given the overarching objective regarding issue of the Environmental Permit, we propose the following lower level objectives for the generic RDD programme into sealing deep site investigation boreholes:

- to advance the scientific understanding of key processes that affect seal performance;
- to understand the extent to which RWMD's illustrative borehole seal concepts are applicable to RWMD's illustrative borehole designs ('up-scaling[1]') and to the range of hydrogeological and hydrochemical environments appropriate to the different 'illustrative' geological settings in the UK;

[1] By 'up-scaling' we mean developing the existing seal design to boreholes that are deeper and have larger diameter than the boreholes for which the seal is currently designed. Principally, this refers to RWMD's B1 and B3 illustrative seal concepts, both of which are currently based on the SKB Basic Seal concept for a post-closure seal. The SKB Basic Seal is designed for 80 mm diameter boreholes up to 1,000m deep. Further RDD would be needed to develop this concept for RWMD's illustrative borehole designs, which are up to 2,000m in depth, and have diameters ranging between 159 mm and 914 mm. See Section2.2.2.

- to identify conditions (if any) where the current RWMD seal concepts are inappropriate or where there is a significant likelihood that the seal concepts cannot be successfully implemented;
- if necessary, to develop alternative seal concepts for those conditions where current RWMD seal concepts are inappropriate or where there is a significant likelihood that the seal concepts cannot be successfully implemented.

The objectives are to be achieved from a programme that is likely to contain the following elements:

- desk-based studies, including modelling;
- laboratory experimental studies and analogue observations, to build understanding of processes and to demonstrate that the existing reference concept can be up-scaled or that viable alternatives exist;
- technology demonstration for key parts of the generic sealing systems. This would probably require demonstration experiments in overseas underground research laboratories and/or surface sites.

We recognise that there is an extensive knowledge base on repository sealing and on borehole sealing from other industries. A lot is known about the materials that could be used for seals and support elements and about interactions between these materials; for example, interface issues between clay and cement or steel. It is important to identify those aspects that are transferrable to borehole sealing, in order to avoid duplication of research. Some of the activities that we identify in this Chapter will therefore not require additional research. Instead, they will use the existing knowledge base and will involve developing arguments that are appropriate to the borehole sealing environment. Other significant activities will include modelling studies, engineering design and work associated with demonstrating seal emplacement.

Optimisation of seals and supports is not a requirement for the generic RDD programme. This has the following consequences for the scope and focus of generic RDD:

- the focus should be to understand the performance that can be achieved by seals and supports under the range of conditions relevant to RWMD rather than to understand the relative importance of sealing boreholes close to or distant from a GDF or to identify less stringent seal concepts for boreholes further from a GDF. The one exception is gas migration, where the potential for gas to migrate towards and into sealed boreholes should be considered[1];
- notwithstanding the above, it will be important to understand the potential range of seal permeabilities required by post-closure assessment for different geological environments and disposal concepts in order to assess the appropriateness of various seal concepts. For example, it might be inappropriate to undertake an extensive R&D programme to develop a seal concept that provided a far higher standard of long-term sealing than was required;
- some seals and supports could be relevant to all geological environments under consideration; for example, they might be suitable for sealing sections of boreholes drilled through cover rocks. All aspects of these seals and supports can be considered in the generic phase of RDD. In contrast, seals for evaporite host rocks are relevant only to the evaporite concept, and might need to be tailored to the

[1] That is, are we confident that there are no mechanisms that would cause gas to move preferentially towards and into sealed boreholes? In such circumstances, could sealed boreholes act as fast pathways for gas to return to the surface?

mineralogy of the evaporite formation at the site under consideration. RDD to address such site-specific issues should be left until the site-specific stage of the RDD programme, unless there are long timescale issues or an issue is identified as being highly important. Generic RDD on evaporite seals should focus on those aspects of the seals that would be common to any evaporite host rock.

In the following Sections, we identify issues for the generic RDD programme on sealing deep site investigation boreholes. Throughout these Sections, we reference back to the evidence base (in particular, the discussions in Sections 4.6 and 5.6) and the outcome of illustrative calculations (Chapter 6) to justify the issues we identify. We first identify issues related to the sealed borehole and its environment, and around demonstrating seal quality (Section 8.2). We then identify issues related to seals (Section 8.3) and supports (Section 8.4). For each component, we consider both material properties and emplacement methods and design.

8.2 The sealed borehole and its environment

RWMD Sealing Objective 2 requires that borehole seals be fit for purpose (Section 2.3). Some seals are installed to ensure that the borehole does not have a significant adverse impact on the long-term environmental safety case for the disposal facility (post-closure seals). Others are installed solely to protect the water resources in the area (water resource seals). For the former, which are the most challenging in terms of performance required, it is necessary to understand the potential range of seal permeabilities required by post-closure assessment for different geological environments and disposal concepts. This would then enable RWMD to assess the appropriateness of various illustrative seal concepts, such as the illustrative concepts presented in Section 2.5, and to be more quantitative in the description of the requirements for the various components in the sealing system (Chapter 7). In this context, we note that illustrative groundwater flow calculations in Section 6.2 indicate that the seal is unlikely to require a permeability equal to that of the undisturbed rock through which the borehole was drilled.

Movement of the rock mass around a sealed borehole could be beneficial or detrimental to the long-term performance of the sealed borehole. See the discussion in Section 5.6.1, which highlights how new flow pathways can be created, depending on the stress state of the borehole walls, or existing flowpaths closed by long-term movements of the rock around the borehole. There is already a substantial knowledge base on the Excavation EDZ around underground openings. This should be used to build understanding of the evolution of the BDZ after the borehole has been sealed, and its potential impact on sealing.

Similarly, the existing knowledge base should be used to build understanding of the extent to which repository perturbations (gas generation and repository resaturation) could affect sealed site investigation boreholes. For example, it would be necessary to determine whether there are any mechanisms that would cause gas to move preferentially towards and into sealed boreholes. The potential for hydraulic and in-situ stress effects following repository resaturation to affect sealed boreholes should also be evaluated.

A key issue for an RDD programme will be to demonstrate how the quality of the emplaced seal is to be determined. Unlike sealing of large structures, such as repository tunnels or galleries, it is not possible to gain man access to sealed boreholes to determine whether sealing materials have been emplaced as planned and have the required properties. Testing and validation is largely confined to measuring material properties at surface, before placing them in the borehole, and indirect testing of the placed material.

As explained in Section 4.3.8, the oil and gas industry undertakes extensive QC at surface to ensure that the mixture of material meets the required standard. During emplacement, the QA is based on measuring the top of each placed seal and comparing it with the expected location based on the injected volumes. However, because it is not practicable to obtain representative samples from the seal after placement, downhole evaluation is limited to pressure tests of seal permeability. The RDD programme should develop a methodology that will ensure that the emplacement and subsequent initial conditions of the seals are as stated by the description of the sealed borehole.

There are some areas where we recommend that no additional RDD is required for borehole sealing:

- radionuclide transport through the sealed borehole. There are no issues for a generic RDD programme because radionuclide interactions with cement and bentonite are well understood, as is the impact of perturbing groundwater chemistry on sorption;
- natural evolution of the geosphere and its impact on sealed boreholes. A number of potential issues were identified in Section 3.4 that could, in certain circumstances, be unfavourable to the performance of the geosphere barrier. We have reviewed these processes and conclude that none require generic RDD through a borehole sealing programme. All should be addressed through RWMD's geosphere research programme.

In summary, key issues are presented in Box 8.1.

Box 8.1 Key generic RDD issues relating to the sealed borehole and its environment

- Determine the potential range of seal permeabilities required by post-closure assessment for different geological environments and disposal concepts in order to assess the appropriateness of various seal concepts
- Understand the likely evolution of the Borehole Damage Zone in potentially relevant geological environments after borehole sealing, and the extent to which such movements in the rock mass surrounding a sealed borehole could be beneficial or detrimental to long-term sealing performance
- Confirm the extent to which repository perturbations (gas generation and repository resaturation) could affect sealed site investigation boreholes
- Develop a QA methodology to demonstrate the quality of the RWMD sealing system
- Determine the extent to which knowledge gained from repository sealing and from other industries is transferrable to sealing boreholes at a GDF site

8.3 Issues and challenges for borehole seals

An important component for a generic RDD programme into sealing deep (i.e. >200m) site investigation boreholes is to understand the extent to which RWMD's illustrative borehole seal concepts are applicable to RWMD's illustrative borehole designs ('up-scaling') and to the range of hydrogeological and hydrochemical environments appropriate to the different 'illustrative' geological settings in the UK. RDD into alternative seal concepts will be required for those conditions where current RWMD seal concepts are inappropriate or where there is a significant likelihood that the seal concepts cannot be successfully implemented.

8.3.1 Post-closure seals in HSR and LSSR

Our recommended functional requirements for post-closure seals are that they provide a long-term seal against key low permeability sections in the host rocks. The standard of sealing required against groundwater flow and gas migration will be informed by the requirements of post-closure performance. Post-closure seals provide this seal for as long as is required by the post-closure Environmental Safety Case. Recent RWMD assessments have been up to a timescale of 1 Ma, so potentially some sealing performance to this timescale is required (see Section 7.4). Given this, we recommend that post-closure seals in HSR and LSSR should be formed from natural materials, as discussed in Section 4.6.2. Bentonite has been extensively researched and used as a borehole sealing material, and has been demonstrated to have both suitably low permeability and high longevity for post-closure seals. We recommend it be used as the material for post-closure seals in HSR and LSSR.

The RWMD illustrative B1 seal concept is based on the SKB Basic Concept for a post-closure bentonite seal. The SKB Basic Concept involves placing blocks of pre-formed high density bentonite in the borehole. To protect the bentonite blocks during emplacement, they are contained in a perforated tube which, in the SKB concept, is formed from copper. We have reviewed borehole seal emplacement methods across a number of industries and conclude that seal materials are generally emplaced as suspensions, slurries, grouts or pellets. The only example of emplacing bentonite as pre-formed blocks in boreholes is provided by the SKB clay seal concept.

Further RDD would be required to develop RWMD's B1 illustrative seal concept to determine whether it could form the generic solution for sealing low permeability zones in both HSR and LSSR. At the present time, it is not clear that the outcome from such RDD would necessarily be successful. We have three broad concerns with an up-scaled SKB Basic Concept for the post-closure seal in HSR and LSSR:

- the practicability of sealing deep boreholes using the 'container' concept to place pre-formed blocks of compacted bentonite. We are concerned that there is a significant risk of the tube becoming stuck in the borehole during placement, particularly in geological environments where boreholes may be less stable and more variable in diameter than those drilled in crystalline rocks by SKB or Posiva. For example, material spalling off the borehole wall could wedge the tube in the borehole;
- that borehole rugosity and the extent of breakouts may mean that the up-scaled SKB Basic Concept is only applicable to limited sections of borehole that require post-closure seals. This would be the case if tubes, which are small enough to pass through overlying in-gauge hole or casing, have to be landed in sections of borehole that have been enlarged through breakout, washout or other mechanisms. Note that sections unsuitable for the B1 seal concept should, in principle, be sealed using the B3 sealing concept;
- that the standard of sealing achievable by an up-scaled SKB Basic Concept might be greater than is actually required.

The RWMD B3 illustrative seal concept is also based on the SKB Basic Concept. It is the equivalent of the B1 seal concept for sections of borehole that are enlarged or where casing has only been locally removed. Because the annular gap between the tube and borehole wall is greater than for the B1 seal concept (see Section 2.5.4), sufficient additional bentonite must be brought into the section to increase the final swelling pressure of the seal. If the up-scaled SKB Basic Concept is to form the basis for a post-closure seal in sections of HSR and LSSR where casing has been locally removed, then RDD will be required to devise a robust approach to placing additional bentonite in the section to be sealed without compromising the location of the copper tube centrally in the borehole and at the correct depth. At the present time it is not clear that the outcome from such RDD would necessarily be successful.

Given these concerns, we believe that the generic RDD programme should contain a strand of work to look at complementary or alternative seal concepts for post-closure seals in HSR and LSSR. We discussed placement of seal materials in Section 4.6.5 and concluded that, across the industries considered, materials are generally emplaced into boreholes as 'suspensions', 'grouts' or 'slurries' using tremie pipes or equivalent. Bentonite pellets (without mineral additives) are widely used in the US to seal oil wells up to 1,000m deep. Bentonite pellets are also used for borehole sealing by some RWMOs; for example, Quellon-HD® is a bentonite – magnetite mixture used as the seal material in the Nagra borehole sealing concept. Bentonite is also widely proposed as a component of the EBS in many repository concepts. A recent report for RWMD [199] reviews a range of emplacement methodologies for clay-based backfills in EBS concepts. These include placement of bentonite as pellets.

The fact that bentonite pellets are considered for use by RWMOs for both borehole sealing and in some EBS concepts demonstrates this placement approach has the potential to guarantee low permeabilities in a range of underground openings, some of which are likely to be irregular. That said, we recognise the difficulties of emplacing pellets in deep boreholes (due to 'bridging' issues) and of accurately placing pellets or slurries. The oil industry may provide solutions that could be relevant for placing materials in deep boreholes at a site for a GDF. Also, the bulk dry density of bentonite pellets will be less than that of pre-formed high density blocks, meaning the final swelling pressure will be lower and permeability higher. Whether such permeabilities will meet the requirements of post-closure seals is a key issue for a generic programme of RDD into sealing deep site investigation boreholes.

We recommend the focus of generic RDD on alternative seal concepts is on alternative approaches to placing the sealant materials in the borehole and on the expected performance of such seals.

The remaining issues for RDD relate to the use of bentonite as the seal material. In all these cases, a substantial knowledge base already exists. A key difference between sealing in the repository near field and sealing boreholes, which we highlighted in Section 5.6, is that the dimensions of a borehole seal are much smaller and the interfacial area with the surrounding rock very high relative to a repository seal. Thus, interactions with the surrounding rocks and groundwater, which might have a small effect on the performance of near-field seals and backfills, may have a much more significant effect on borehole seals. The implications of this need to be addressed in the generic RDD programme.

The issues fall into the following broad categories:

- understanding the conditions for onset of bentonite erosion by flowing groundwater in the range of groundwater and geological environments of potential relevance to RWMD. See Section 5.2.2.6 for discussion. We recognise the ongoing programme of work under the BELBaR project, and the work that has been undertaken in Sweden and Finland to understand the conditions for the onset of bentonite erosion at the particular sites being considered. However, a broader understanding is needed should these sealing concepts be developed for other geological environments;

- determining the permeability of bentonite, as a function of swelling pressure, in a range of groundwater environments of potential relevance to RWMD. This will enable calculation of seal permeability for different groundwater chemistries and emplacement methods (the emplacement method effectively determines the mass of bentonite that can be introduced to the section, which is one influence on equilibrium swelling pressure). An extensive knowledge base already exists; it may be possible to extrapolate from existing information to calculate the relationship between permeability and swelling pressure for all groundwater environments of potential relevance to RWMD;
- longevity of bentonite in natural systems. Extensive research has already been carried out (see, for example, Section 5.2.2 and Section 5.6.1, which generally demonstrate the stability of bentonite in natural systems over geological timescales), and it is unlikely that further general R&D on the stability of bentonite in groundwater systems would be appropriate. However, because of the small volume of a bentonite borehole seal and the large relative surface area in contact with groundwater, it would be appropriate to confirm whether limited reactions at the seal – rock interface could impact on seal performance;
- the merits or otherwise of using mixtures of bentonite with other materials (such as magnetite in Quellon-HD®) and the consequences of long-term interactions that could occur within a bentonite-based seal through reactions between components. In Section 4.6.6, we highlight concerns that mixtures can compromise the way the individual sealing materials work and, because they have potential for density segregation and particle aggregation during placement, could lead to the formation of heterogeneous barriers. We also highlight the potential for interactions between chemically incompatible materials; whilst these are not expected to result in significant changes to seal properties over engineering timescales, longer-term sealing performance might be compromised. See Section 8.4.1 for further discussion;
- understanding the interactions of bentonite with any casing that remain in the borehole.

As part of the process to identify issues and challenges for bentonite seals, we have identified a number of features, events or processes where arguments can be made to demonstrate that there are no significant impacts on seal performance. For example:

- resaturation times for bentonite seals. Bentonite seals need to be fully resaturated to perform their function. Where water ingress to the sealed section is slow, resaturation times will be increased. In the limit, if no water flows into the sealed section, the bentonite seal will not swell. In these circumstances lack of swelling is not an issue, because there are no flows to seal against;
- at 2,000m depth (the maximum depth considered in this report), maximum ambient temperature is likely to be approximately 90℃; average temperature at this depth is likely to be approximately 60℃. See Section 3.3.5. These temperatures are unlikely to significantly affect the chemical evolution of the sealing materials.
- Further, extensive research on the performance of clay-based and cement-based materials in repository near field conditions, where they may be exposed to significantly higher temperatures than in boreholes, has already been undertaken.

In summary, key issues are presented in Box 8.2.

Box 8.2 Key generic RDD issues relating to post-closure seals in HSR and LSSR

- Determine whether RWMD's B1 and B3 illustrative seal concepts (the up-scaled SKB Basic Seal concept and a variant of this approach) are potential solutions for post-closure seals in all potentially relevant HSR and LSSR
- Develop a complementary or alternative sealing concept for post-closure seals in HSR and LSSR. Generic RDD should consider the feasibility of these approaches for placing seals and the expected performance of such seals
- Further develop understanding of the performance of bentonite in borehole seals. For all these aspects considered, a substantial knowledge base already exists
- Further develop understanding of the longevity of bentonite in borehole seals. For all these aspects considered, a substantial knowledge base already exists.

8.3.2 Post-closure seals in evaporites

More than any other geological environment, understanding of the long-term performance of borehole seals in evaporites should take account of the movement ('creep') of the rock around the borehole. This movement of the rocks around the seal could mitigate the effects of any shrinkage in the seal. An aspect that is unique to seals in evaporites is the need to exclude groundwater from the system. Thus, there may be a requirement to place an additional long-lived seal at the potentially vulnerable boundary of the post-closure evaporite seal to protect against groundwater ingress to the seal (in particular, where the post-closure seal is itself formed of evaporite minerals).

Any evaporite seal concept is likely to involve the pumping of slurries or crushed material rather than trying to emplace a solid material. Issues are as discussed for support elements in Section 8.4.

Two approaches have been taken to the design of seals for evaporite formations: seals formed from natural evaporite minerals and seals formed from salt-saturated cements. RWMD's illustrative C-SS seal concept is based on the latter approach. We recommend that any generic RDD into post-closure seals in evaporites considers both of these approaches. The long-term performance of seals from natural materials may be easier to demonstrate than the performance of seals formed from salt-saturated cement.

The composition of evaporite seals (both those formed from natural evaporite minerals and from salt-saturated cements) would depend on the site evaporite mineralogy. For this reason RDD to design such seals should be left until the site-specific stage of the programme unless there are long timescale issues or an issue is identified as being highly important. At the present time, we identify neither long-timescale nor highly important issues that would require generic RDD. Issues associated with salt-saturated cements are around uncertainties in their long-term performance.

In summary, key issues are presented in Box 8.3.

Box 8.3 Key generic RDD issues relating to post-closure seals in evaporites

- Consider an alternative seal concept in addition to RWMD's C-SS concept, which is based on salt-saturated cement
- Build understanding of the long-term performance of salt cement

At the present time, we identify neither long-timescale nor highly important issues associated with the performance of post-closure evaporite seals formed from evaporite minerals that would require generic RDD.

8.4 Issues and challenges for support elements

8.4.1 Support element for lower permeability sections of borehole

Support elements could potentially be used in any host rock and in the overlying cover rocks. This Section considers support elements to be used in the lower permeability sections of the borehole. The RWMD illustrative seal concept for this application is B2. In the illustrative RWMD borehole sealing system, B2 is to be deployed as a support component in lower permeability rocks; C1 is to be deployed as a support component in higher permeability rocks. The permeability/transmissivity boundary between these two support components (B2 and C1) needs to be established.

There is a range of materials that would meet the requirements for a support element in lower permeability sections of borehole, which we have described in Chapter 4. In particular, see the discussion in Section 4.6. For example (and in no particular order):

- pure cement (with additives and supplementary cementing materials as appropriate), which is commonly used in the oil industry;
- barite-based materials, such as used by Nagra at Wellenberg and by the oil and gas industry (SANDABAND®) to seal wells;
- crushed natural rock mixtures, designed to mimic (as far as is required) the permeability of the formation in which it is placed;
- bentonite-quartz mixtures;
- cement-bentonite mixtures, which are commonly used for water resource protection.

The issues with regards to performance of support elements for post-closure seals are twofold. Both relate to the advantages and disadvantages of various materials:

- mechanical stability. For example, if mixtures are to be used, would any long-term interactions between the components (such as between bentonite and cement) impact on the long-term mechanical stability of the support element? Likewise, the potential erosion of bentonite from bentonite-containing mixtures (such as bentonite-quartz and SANDABAND®) would need to be understood. In such mixtures, the grading of the sand would have to be designed to inhibit movement of bentonite. In the case of pure cement, which we propose as a support rather than a seal, the only issue to be considered will be around potential volume changes as the cement evolves; these changes are unlikely to be significant;

- chemical interactions with adjacent clay seals. Such interactions (Section 5.2.2.6) might lead to mineralogical and/or chemical changes that might reduce the longevity of the clay seal. The nature of the reactions between cement and bentonite is well-understood and extensive experimental, modeling and natural analogue studies have been carried out. Of particular relevance to borehole sealing is to understand the spatial scale of any interactions within the seal and the changes to hydraulic properties that take place. Calculations in Section 6.3.4 indicate that reactions between cementitious support elements and adjacent bentonite seals are unlikely to lead to alteration of the bentonite over distances of more than a few tens of centimetres. One approach to mitigate the effect of some interactions would be to place a greater length of clay seal than is required, and to accept that some of this seal is 'sacrificial'.

In general, we believe there are fewer issues or challenges associated with emplacement of support elements than with some post-closure seals. Any concept for support elements in lower permeability sections of borehole is likely to involve pumping or placing crushed material rather than trying to emplace blocks of pre-formed solid material. Extensive oil and gas experience is relevant to this method of emplacement. For example, Section 4.6.5 describes how bentonite pellets (without mineral additives) are widely used in the US to seal oil wells up to 1,000m deep. Bentonite pellets are also used as the emplacement method for some RWMO applications; for example, Quellon-HD® is a bentonite – magnetite mixture used as the seal material in the Nagra borehole sealing concept. Notwithstanding this, there are a number of issues around placing material as slurries or pellets, which we discussed in Section 8.3.1.

From an oil industry perspective, the focus during the placement of the support element would be the avoidance of any channels or micro-annuli from the onset, and the effective isolation of any permeable zone from the onset, rather than any risk of subsequent erosion through a barrier. If erosion or solution of any adjacent post-closure seal were to be deemed a potential risk, the support might need to be modified to prevent or significantly restrict any fluid flow towards the seal, for example by the placement of additional materials at the interface. A similar solution might be sought if the extent of chemical interaction between the support element and any adjacent seal was deemed to be detrimental to the long-term performance of the seal.

In summary, key issues are presented in Box 8.4.

Box 8.4 Key generic RDD issues relating to support element for lower permeability sections of borehole

- Establish the permeability/transmissivity boundary between use of support components for lower and higher permeability sections of borehole
- Identify advantages and disadvantages of potential materials for the support element. The two principal issues are the mechanical stability of the support element over long time periods and chemical interaction with adjacent seals
- Identify any requirements to place additional materials at the interface with adjacent seals, for example if erosion or solution of any adjacent post-closure seal were to be deemed a potential risk. This is an issue particularly for evaporites

8.4.2 Support element for higher permeability sections of borehole

This section considers support elements to be used in the higher permeability sections of the borehole. The RWMD illustrative seal concept for this application is C1. As discussed in Section 8.4, the permeability/transmissivity boundary between this support element and the support element for use in lower permeability sections of borehole needs to be established.

As with support elements for lower permeability sections of rock, the emplacement method is likely to involve pumping or placing crushed material rather than trying to emplace blocks of pre-formed solid material. Extensive oil and gas experience is relevant to this method of emplacement. As with the support element for lower permeability sections of borehole, there is a range of materials that would meet the functional requirements. For example:

- quartz sand, with additional cement or other material (such as a small component of bentonite) if a low permeability at the time of borehole sealing is required to prevent damage from inflows/outflows as overlying seals are placed;
- crushed natural rock mixtures, designed to mimic (as far as is required) the permeability of the formation in which it is placed.

As with the support element for lower permeability sections of borehole, the generic RDD programme needs to consider the advantages and disadvantages of various compositions with regards to mechanical stability and chemical interactions with adjacent clay seals. Such interactions might occur if cement is added to the material. In addition, any requirement for low permeability at the time of borehole sealing needs to be established. This may result in a maximum permeability being defined for the support element at the time of borehole sealing.

In summary, key issues are presented in Box 8.5.

Box 8.5 Key generic RDD issues relating to support element for higher permeability sections of borehole

- Establish the permeability/transmissivity boundary between use of support components for lower and higher permeability sections of borehole
- Identify advantages and disadvantages of potential materials for the support element. The two principal issues are the mechanical stability of the support element over long time periods and chemical interaction with adjacent seals
- Establish any requirements for low permeability at the time of borehole sealing

9 Recommended programme of generic RDD into sealing deep site investigation boreholes

9.1 Introduction

In this Chapter, we recommend a programme of generic RDD into sealing deep (>200m) site investigation boreholes. We have structured the generic RDD programme by issue (see Chapter 8), and also indicate the types of activities that we expect will be needed to address the issue.

In Section 9.2, we identify early RDD activities ('stage 1'). These are shown in the top part of Figure 9-1 and include completing the functional requirement specification (if needed), modelling to define the expected flow regimes and requirements on seal performance, developing some aspects of conceptual understanding and an evaluation of whether RWMD's B1 and B3 seal concepts are potentially appropriate solutions. It also includes a review on where progress beyond the current 'state of the art' is needed in terms of transferability from other fields (e.g. emplacement feasibility, longevity, etc).

A Hold Point at the end of the first stage of generic RDD activities is recommended, to enable refinement of the second stage of the generic RDD programme (Sections 9.3 and 9.4) if appropriate. The second stage of the generic programme involves RDD activities for individual seal/support elements to address the issues identified (Section 9.3). Generic RDD to demonstrate seal quality is presented in Section 9.4.

Three major issues are identified from Chapter 8:

- concerns that RWMD's illustrative B1 and B3 seal concepts may not be appropriate in some geological environments potentially relevant to RWMD. This leads to a recommendation that the generic RDD programme contains a research strand to develop complementary or alternative seal concepts;
- a requirement to determine the post-closure performance requirements for borehole seals in a range of geological environments;
- a need to develop and test a QA methodology and demonstrate the quality of an emplaced borehole seal. This work might also identify issues that would result in recommendations for borehole design.

Our recommended high-level workflow is shown in Figure 9-1. RDD activities concerned with individual seal and support elements are shown in Figure 9-2. Note that Figure 9-2 presents activities, not a workflow. It is possible that several activities under each heading could be undertaken in parallel. More detailed description of proposed RDD activities are given in Section 9.2 to Section 9.4. Again, note that some activities may be undertaken in parallel.

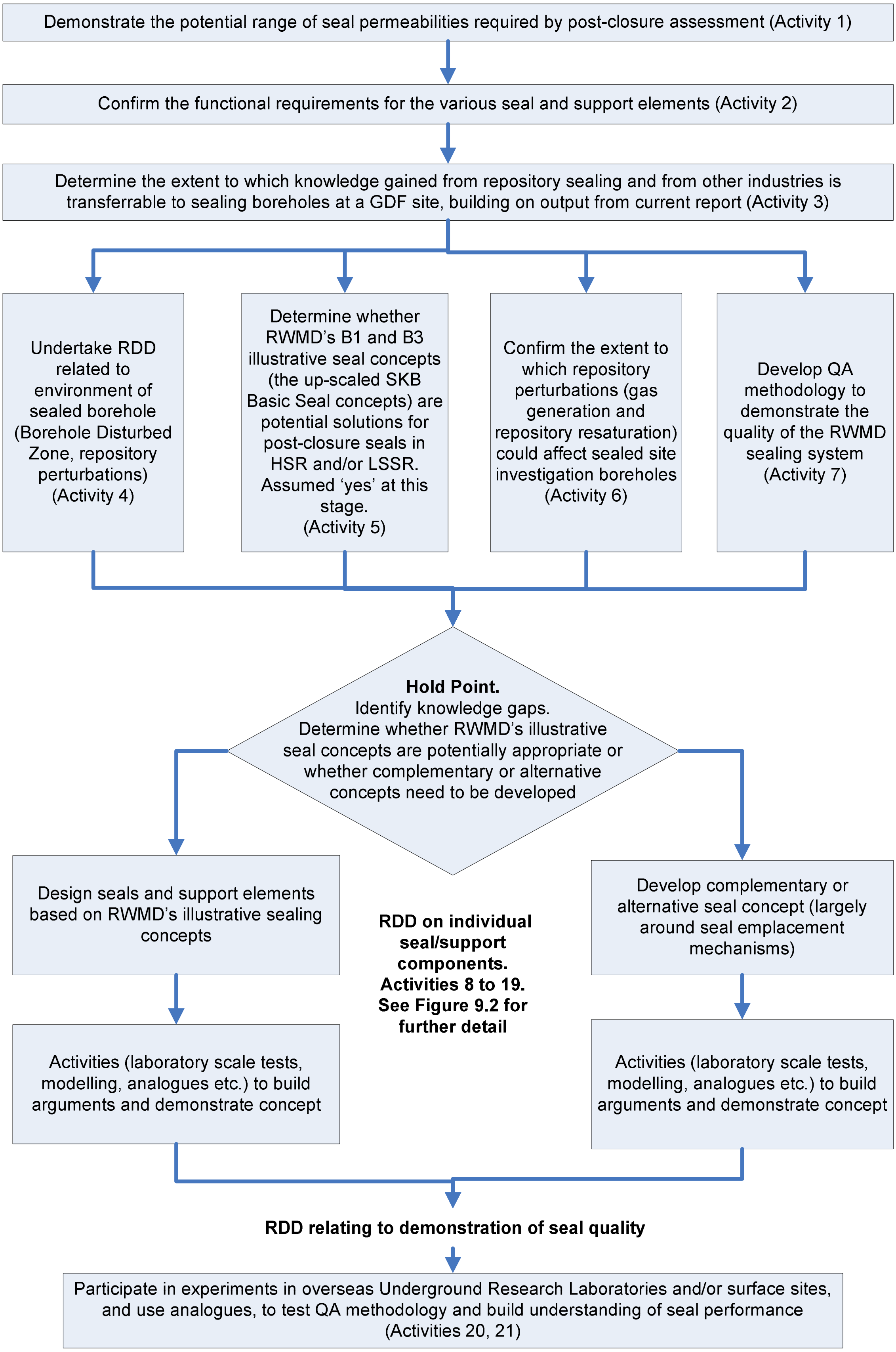

Figure 9-1 Proposed high-level workflow for a generic RDD programme into sealing deep (>200m) site investigation boreholes. 'Activities' relate to activities presented in Sections 9.2 to 9.4.

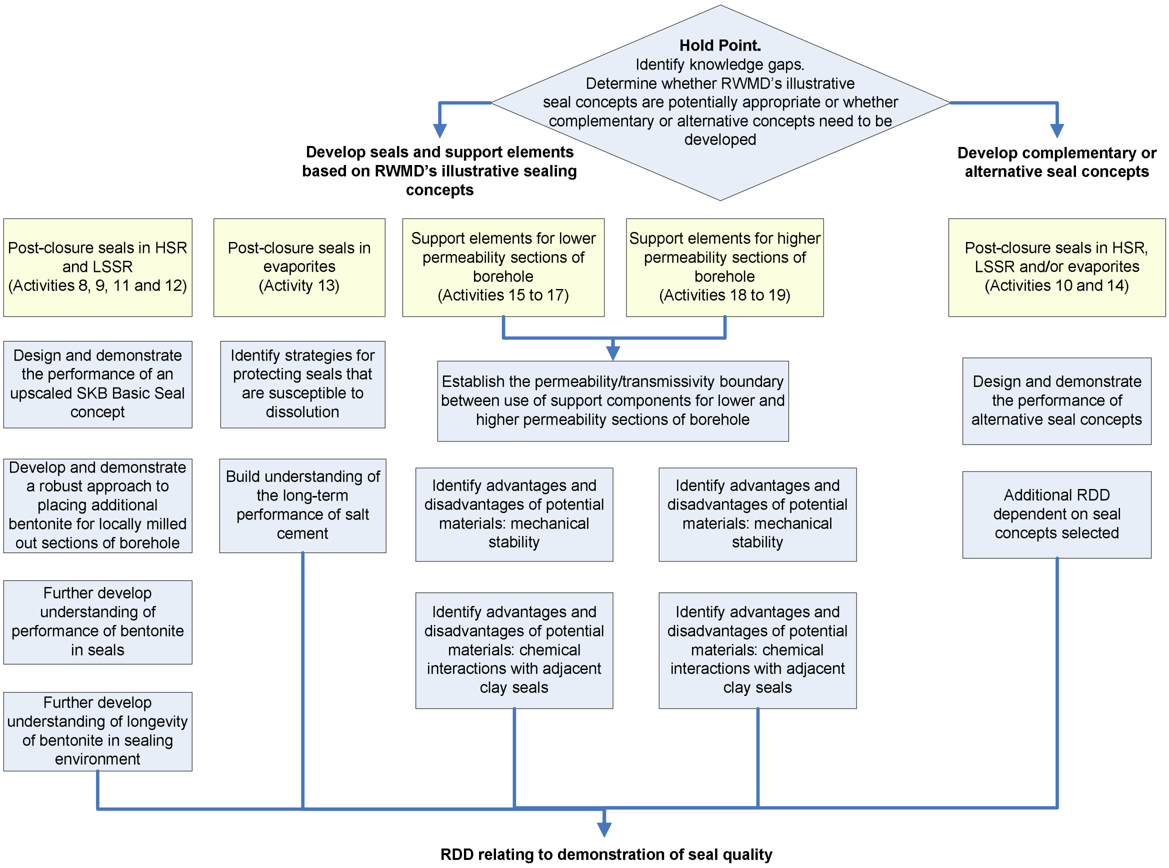

Figure 9-2 Detail of generic RDD programme into sealing deep (>200m) site investigation boreholes: RDD on individual seal/support elements. Note this presents activities, not a proposed workflow. 'Activities' relate to activities presented in Sections 9.2 to 9.4.

9.2 Stage 1 RDD activities, leading to project Hold Point

Areas for RDD are listed below.

1. Activity 1. Demonstrate the potential range of seal permeabilities required by post-closure assessment for different geological environments and disposal concepts in order to assess the appropriateness of various seal concepts

This activity would have the following scope:

- develop a numerical model of a section of sealed borehole to confirm the simple scoping calculations and conclusions presented in Section 6.2. Understand the relative importance of flows through the seal, the interface with the rock, the BDZ and the surrounding undisturbed rock;
- develop storyboards/conceptual models, with parameter ranges (potentially based on those in Chapter 3), for borehole sealing in the various geological environments;
- use the storyboards/conceptual models to generate numerical models of simplified representations of the three illustrative geological environments: HSR, LSSR and evaporites, all overlain by cover rocks.

- modelling should demonstrate the overall impact of sealed boreholes on geosphere performance. This would include modelling to understand how the groundwater flux will be affected by (i) permeability of the post-closure seals, (ii) different proportions of seals and supports and (iii) different geological environments. The key output would be a comparison of groundwater fluxes through the geosphere in the presence and absence of the sealed borehole, which would build understanding of the effect of sealing concepts and standards of sealing on geosphere containment functions;
- from the above, identify ranges of seal performance commensurate with maintaining the containment function of the geosphere for each illustrative geological environment.

2. Activity 2. Confirm the functional requirements for the various seals and supports for the RWMD borehole sealing system and elicit ranges of hydraulic properties for various seal and support concepts at placement and at various times after placement

This report recommends functional requirements for the various elements (seals and supports) of RWMD's borehole sealing system. A workshop, with RWMD and appropriate experts, should be held to consider whether these recommendations are appropriate. This workshop could consider whether the list of functional requirements identified in Section 7 is adequate. Ranges for the hydraulic properties of the different conceptual seals and supports at placement and at various times (e.g. 100 years, 1,000 years, 10,000 years and 100,000 years) after placement should be elicited, and supported by reasoned arguments. These ranges should be used in subsequent modelling activities. The ranges should be periodically reviewed in light of the subsequent RDD activities undertaken, and refined as necessary. Modelling should be repeated as necessary in light of any significant changes.

3. Activity 3. Determine the extent to which knowledge gained from repository sealing and from other industries is transferrable to sealing deep site investigation boreholes at a GDF site

This desktop consultancy activity would determine the extent to which knowledge gained from repository sealing and from other industries is transferrable to sealing deep site investigation boreholes at a GDF site. We are aware that a large knowledge base exists, which should be built on rather than duplicated. This proposed RDD activity would build confidence in the recommendations for generic RDD made in the current report. Data gaps, where the information is not transferrable, will be identified. Further work might take the form of modelling, experiments (laboratory- and/or field-scale) and analogue studies. Even where information is transferrable, it will generally be necessary to use this information to develop a description, or position statement, specific to the sealed borehole.

The RDD on borehole sealing that is recommended in this report will be undertaken as part of RWMD's research programme, which is described in [200]. The research programme is structured into a number of 'topic areas', shown in Figure 9-3. Research relevant to backfill and buffers is being undertaken principally in the Near-field Evolution area; gas and radionuclide migration through backfill and buffers are considered in the Gas and Radionuclide Behaviour topic areas respectively. Interactions between backfill/buffers and the geosphere are considered in the Geosphere topic area.

Some issues for sealing deep site investigation boreholes that we identified in Chapter 8 are already being addressed through other parts of the RWMD research programme or, if not, would be better addressed through those topic areas rather than through a separate borehole sealing RDD programme. In our recommendations in the following sections, we make it clear where we believe future activities should be addressed through other parts of the RWMD research programme.

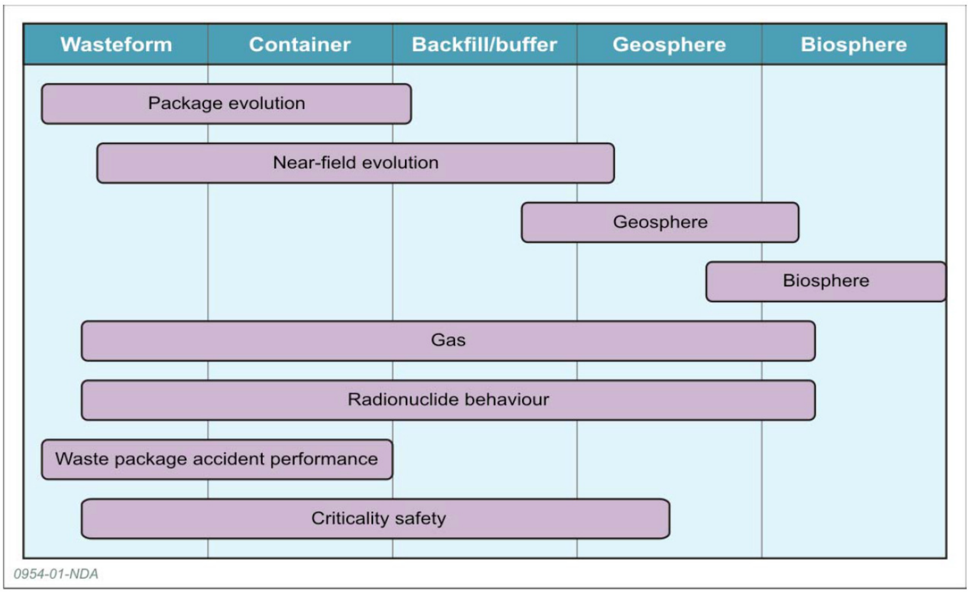

Figure 9-3 Topic areas for the RWMD Research programme

4. Activity 4. Use the existing knowledge base to understand the likely evolution of the Borehole Damage Zone in potentially relevant geological environments after borehole sealing, and the extent to which such movements in the rock mass surrounding a sealed borehole could be beneficial or detrimental to long-term sealing performance

This activity would involve consultancy and scoping calculations, and would have the following scope:

- use the existing knowledge base (e.g. from RWMOs and the oil and gas industry) to develop appropriate conceptual models for BDZs;
- use the existing knowledge base to identify the circumstances where fractures could develop in the seal. For example, the presence of smectite minerals in clay seals provides ductility and swelling; such seals could only fracture in the event that reaction with cementitious fluids resulted in significant mineralogical alteration;
- use the existing knowledge base to understand the likely evolution of the BDZ in a range of relevant geological environments after borehole sealing;
- use the above (development of the BDZ and fracturing in the seal) to determine the extent to which rock movements could be beneficial or detrimental to long-term sealing performance;
- identify any issues for borehole design.

5. Activity 5. Determine whether RWMD's B1 and B3 illustrative seal concepts (the up-scaled SKB Basic Seal concept and a variant of this approach) are potential solutions for the post-closure seals in all potentially relevant HSR and LSSR

This desk-based activity is intended to determine whether it would be impracticable or unnecessarily onerous to implement RWMD's illustrative B1 and B3 seal concepts in boreholes that are (i) deeper and have larger diameter and (potentially) higher rugosity than boreholes currently considered by SKB or Posiva and (ii) are constructed in a range of potentially relevant HSR and LSSR environments. The following should be addressed:

- the ease of emplacement and the time required to place the seals;
- the risks of the perforated copper tube becoming stuck in the borehole during placement, and identification of solutions to reduce this risk to acceptable levels;
- the practicability and risks of introducing additional bentonite prior to placement of a perforated tube containing compacted bentonite, and identification of any potential solutions;
- when it is appropriate to use RWMD's B3 illustrative seal concept. Recommendation on the boundary between use of B1 and B3 illustrative concepts should be made;
- the likely relative uses of RWMD's B1 and B3 illustrative seal concepts in the range of borehole conditions that might be encountered by RWMD. This would require a review of the variability in borehole diameter in potentially relevant geological environments. This activity should also consider the implications of different drilling techniques on the nature of the borehole wall, as the technical challenge and cost of sealing a borehole to a particular standard may be strongly influenced by the approach to construction;
- the standard of sealing achieved in comparison to the potential requirements of post-closure performance.

At the end of this activity, it will be possible to say whether RWMD's B1 and B3 illustrative seal concepts remain as potential solutions for post-closure seals in all or some of the potentially relevant HSR and LSSR.

Some Stage 2 activities will be dependent on the outcome from Activity 5. If it is concluded that up-scaled SKB concepts are potential solutions for post-closure seals in HSR and/or LSSR, then Activities 8 and 10 below will be undertaken in parallel (see also Figure 9-1). If, on the other hand, the up-scaled SKB concepts were considered impracticable or unnecessarily onerous to implement in both HSR and LSSR environments, then Activity 8 below will not be required and more emphasis would be placed on Activity 10.

6. Activity 6. Confirm the extent to which repository perturbations (gas generation and repository resaturation) could affect sealed site investigation boreholes

These modelling and consultancy activities would have the following scope:

- determine the potential for GDF-derived gas to migrate towards and through sealed boreholes. The object of this modelling task would be to determine whether there are any mechanisms that would cause gas to move preferentially towards and into sealed boreholes. In such circumstances, modelling and the existing knowledge base would be used to determine whether sealed boreholes (including the BDZ) could act as fast pathways for gas to return to the surface. An extensive knowledge base on gas migration through EBS and rocks exists (for example, the FORGE[1] project [201]), and should be used to inform the RDD activities. The requirement for further RDD would depend on the outcome from this activity;

[1] This project has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no 230357

- determine the potential for the hydraulic and in-situ stress effects following repository resaturation to affect sealed boreholes. The existing knowledge base (e.g. from RWMOs and the oil and gas industry) would be used to develop appropriate conceptual models, which would then be tested.

7. Activity 7. Develop QA methodology to demonstrate the quality of the RWMD sealing system

The RDD programme should develop a methodology that will ensure that the emplacement and subsequent initial conditions of the seals are as stated by the description of the sealed borehole. Where possible, this will draw on experience from QA methodologies developed in other industries and programmes that have already built confidence in (for example) emplacement technologies and seal performance.

This task could also usefully consider whether techniques can be developed to demonstrate the quality of the emplaced seal using borehole tools (as Section 4.3.8 makes clear, there are currently no logging tools or technologies available to the oil industry that might provide any look-ahead capability to 'see' into the plug using acoustic, resistivity or density techniques).

Prior to borehole sealing, requirements for additional pre-sealing surveys need to be identified. The rationale for such surveys is presented in Section 2.4.4. A generic RDD programme needs to consider these issues and come up with a solution. For example, it may appropriate to develop a flowsheet, with supporting justification, to ensure that all necessary surveys are undertaken prior to sealing.

Hold Point
Following completion of the above tasks, it would be necessary to review the planned RDD to be undertaken on individual seal and support components.

9.3 Stage 2 RDD activities on individual seal/support elements

9.3.1 RDD relating to post-closure seals in HSR and LSSR

The current RWMD illustrative concepts for post-closure seals in HSR and LSSR (B1 and B3) are based on the SKB Basic Concept. The SKB Basic Concept is designed for 80 mm diameter boreholes up to 1,000m deep in HSR. Currently, it has only been emplaced at a depth of 551m (see Section 4.2.1.2).

The work to be undertaken in Activities 8 and 10 will depend on the outcome of Activity 5. If it is concluded that the up-scaled SKB Basic Concept is a potential solution for post-closure seals in HSR and/or LSSR, then Activities 8, 10 and 10 below will be undertaken in parallel (see also Figure 9-1 and Figure 9-2). If, on the other hand, the up-scaled SKB concepts were considered impracticable or unnecessarily onerous to implement for both environments, then Activities 8 and 9 below will not be required and more emphasis would be placed on Activity 10.

8. Activity 8. Design and demonstrate the performance of an up-scaled SKB Basic Seal concept

The following RDD will be required and solutions will need to be found if the SKB Basic Concept is to be developed as a generic solution for RWMD's post-closure seal in HSR and/or LSSR. These modelling, desk-based consultancy and laboratory activities would have the following scope:

- design an up-scaled SKB Basic Concept for use in larger, deeper boreholes with higher rugosity than that encountered by SKB or Posiva. The consequence of the higher rugosity is that a bigger annular gap would be required between copper tube and borehole wall in order to reduce the risk of the tube becoming stuck in the borehole as it was lowered into position. The design, which will build on the outcome from Activity 3, will require solutions to be found for:
  - centralising the tube in the section of borehole to be sealed and;
  - reducing the risk of the tube becoming stuck in the borehole during placement to acceptable levels, particularly in geological environments where boreholes may be less stable and more variable in diameter than those drilled by SKB or Posiva.
- understand whether bentonite loss from up-scaled tubes during placement is any different for that in the SKB Basic Concept;
- undertake modelling studies to understand whether the larger annular gap has any consequences on seal performance. For example:
  - determine the swelling pressure theoretically achieved by the seal in a range of groundwater environments of potential relevance to RWMD. Use the existing knowledge base to estimate the permeability of the up-scaled seal under this range of conditions;
  - model the evolution of swelling within the bentonite to determine whether there are constraints to the movement of bentonite from the perforated tube into the surrounding rock that might preclude or unduly delay homogenisation of sealing pressure in the section. This would build on the coupled modelling already undertaken to understand bentonite behaviour in HLW/SF emplacement holes;
- undertake laboratory experiments to demonstrate the development of the seal as the bentonite swells and is extruded from the copper tube into the annular gap between tube and borehole wall. (Laboratory and field experiments to demonstrate the performance of the SKB Basic Seal Concept is presented in Section 4.2.1.) Such experiments would be used to build understanding , and hopefully, confidence, in the up-scaled sealing concept;
- identify the conditions where corrosion of copper can occur. A generic RDD programme should reach a position on the potential for copper corrosion in the range of potentially relevant groundwater conditions, and its potential impact on B1 seal longevity. This activity is expected to use the existing knowledge base from SKB's research programme, rather than to involve further research by RWMD.

9. Activity 9. Develop and demonstrate a robust approach to placing additional bentonite before placing the perforated tube in sections of borehole where the casing has locally been milled out

- This design and laboratory experimental activity would determine whether a robust solution can be found for placing additional bentonite in sections of borehole where the casing has locally been milled out. It should include laboratory experiments to demonstrate the concept.

10. Activity 10. Develop a complementary or alternative sealing concept for post-closure seals in HSR and/or LSSR

The generic RDD programme should contain a strand of work to look at complementary or alternative seal concepts for post-closure seals in HSR and/or LSSR. The focus should be on alternative approaches to placing the sealant materials in the borehole. In Section 8.3.1, we identified potential alternative approaches to placing seals; 'suspensions', 'grouts' and 'slurries'. We recognise the difficulties of emplacing pellets in deep boreholes (due to 'bridging' issues) and of accurately placing pellets or slurries, and therefore these issues should be addressed. The oil industry may provide solutions that could be relevant to sealing deep boreholes at a site for a GDF. For example, there may be potential to place pelleted bentonite using the dump bailer method (i.e., using a wireline-conveyed bailer or coiled tubing-conveyed bailer) to carry solids to the bottom of a hole, as is sometimes used for gravel packing oil and gas wells. Runs could be repeated as necessary until sufficient material was emplaced. The advantage of the approach is that a known volume of pellets can be accurately placed.

If it was decided that the SKB Basic Concept was not an appropriate concept for post-closure seals in HSR and/or LSSR, then further work would also be required to determine the permeability of bentonite as a function of swelling pressure in a range of groundwater environments of potential relevance to RWMD. The bulk dry density of bentonite pellets will be less than that of pre-formed high density blocks, meaning the final swelling pressure will be lower and permeability higher. Whether such permeabilities will meet the requirements of post-closure seals is a key issue for a generic programme of RDD into sealing deep suite investigation boreholes (see Activity 1).

Modelling and use of the existing knowledge base are the recommended approaches to generate understanding of seal permeability for different groundwater chemistries and emplacement methods (the emplacement method effectively determines the mass of bentonite that can be introduced to the section, and hence the density when water-saturated, which is one influence on equilibrium swelling pressure).

11. Activity 11. Further develop understanding of performance of bentonite in borehole seals

We recognise that an extensive knowledge base already exists. The tasks to be undertaken as part of this activity will be influenced by the outcome of Activity 3. Only where knowledge gaps exist, or where information and understanding from other areas is not transferrable, will further research be required. Based on our reviews and experience, we identify a number of RDD activities under this topic.

- SKB is undertaking a substantial programme of work to define the conditions under which bentonite starts to be eroded by flowing groundwater within specified ranges of groundwater salinity/chemistry. This activity would build on the SKB work and, as necessary, extrapolate the approach to address the range of groundwater chemistries and flow rates of potential relevance to RWMD;
- understanding the influence of mixing inert quartz sand with the bentonite on the potential for erosion of bentonite. Any potential benefits should be evaluated, by review of existing literature.

12. Activity 12. Further develop understanding of longevity of bentonite in the borehole sealing environment

We recognise that an extensive knowledge base already exists, both on the behaviour of bentonite in natural systems and on the interactions of bentonite with other materials, principally cement and steel, that might occur in the EBS of a GDF. The tasks to be undertaken as part of this activity will be refined by the outcome of Activity 3. Based on our reviews and experience, we identify a number of RDD activities under this topic:

- reach a position on the importance of interactions of bentonite with any casing that remains in the borehole. We note that bentonite and casing will largely be in direct contact inside sections of casing left in place in the borehole. This should not impact on the quality of the seal with the surrounding rock unless the length-scale of any interaction is large;
- identify any interactions that could occur through the use of mixtures of bentonite with other materials (such as magnetite in Quellon-HD®). Such interactions are likely to be less significant than those with corroding steel;
- identify any interactions with groundwater. The existing understanding on illitisation should be summarised, and arguments made as to why illitisation of bentonite in borehole seals will not be significant.

RDD to understand interactions of bentonite with other borehole sealing or support materials is presented in Section 9.3.3.

9.3.2 RDD relating to post-closure seals in evaporites

The main activities at the generic stage of the RDD programme will be as follows.

13. Activity 13. Identify strategies for protecting seals that are susceptible to dissolution

This activity would use the existing knowledge base to identify seal materials that could be used to form long-lived low permeability seals against the potentially vulnerable surface of post-closure seals and evaporite formations that are susceptible to dissolution. The activity would conclude by identifying placement strategies for such materials. It is possible that the conclusion will be that post-closure seals for HSR and LSSR are appropriate for this purpose.

14. Activity 14. Build understanding of the long-term performance of salt cement

Salt concretes are used extensively in the oil and gas industries for sealing boreholes in subterranean evaporite formations. Extensive consideration is given to (for example, see [202]):

- evaporite formation effects on the cement slurry;
- evaporite formation effects on the set cement seal;
- effects of salts added to the cement by design.

An activity to review the evidence base on this subject and identify any areas for subsequent RDD is proposed. The focus should be on understanding how the above issues might affect the longevity of salt-saturated cements. RDD to understand implications for long-term creep around borehole on sealing performance is included in Activity 2. We note that the mineralogy of the evaporite to be sealed is not known at the generic stage, and that the mineralogy of the evaporite (for example, variable amounts of soluble magnesium and sulphate minerals) is likely to impact on the first two bullet points above. The lower strength of salt-saturated cements and their slower strength build up is one issue to be considered under the third bullet point.

We note that the RWMD Near-field Evolution topic area is already undertaking research into the long-term evolution of cements. The cement-related RDD identified above could be undertaken through the Near-field Evolution area; it would not be appropriate to initiate RDD on cement evolution through the borehole sealing project.

9.3.3 RDD relating to support elements for lower permeability sections of borehole

There are two distinct RDD activities relating to support elements for lower permeability sections of borehole. The first is to establish the permeability/transmissivity boundary between the use of this support element and the support element for higher permeability sections of borehole. The second is concerned with material properties for support elements for lower permeability sections of borehole and with interactions between these materials and adjacent clay-based seals. RDD on placement techniques would be covered by Activity 10.

15. Activity 15. Establish the permeability/transmissivity boundary between use of support components for lower and higher permeability sections of borehole

- This task should develop arguments for where the permeability/transmissivity boundary should lie, based largely on the requirements for water resource protection;
- As appropriate, modelling (further to Activity 1) should evaluate the consequences of using different proportions of the two support elements in borehole sealing concepts. Estimates of the as-placed and long-term hydraulic conductivity of support components for lower and higher permeability sections of borehole will be required.

16. Activity 16. Identify advantages and disadvantages of potential materials for the support element for lower permeability sections of borehole: mechanical stability

Because of the extensive existing knowledge base, only limited RDD might be required.

- if mixtures are to be used, RDD should identify any long-term interactions between the components (such as between bentonite and cement) that might impact on long-term mechanical stability;
- the potential erosion of bentonite from bentonite-containing mixtures (such as bentonite-quartz and SANDABAND®) would need to be understood;
- if bentonite-sand was to be identified as a strong contender for the support element, then the potential exists for using natural bentonite as the material, rather than to produce an artificial mixture prior to placement (with the consequent requirement to ensure thorough mixing of the two components). In natural bentonite, the clay (phyllosilicate) -silica ratio varies from almost pure montmorillonite (e.g. Wyoming) to silica-rich. It would therefore be possible to choose a material to suit the site requirements;
- in the case of cementitious materials, which we propose as a support rather than a seal, the principal issue to be considered will be around potential volume changes as the cement evolves. These changes are unlikely to be significant, but RDD should

confirm this. Arguments regarding the long-term permeability that could be ascribed to cement supports should be developed. Potential activities include:

- identify what cement formulations could be most appropriately used in each of the geological environments of potential interest (also see Activity 14);
- calculations (cf. [203]) and analogue observations to assess if carbonation could play a significant role in minimising cement plug degradation via external armouring. Currently, no directly relevant natural analogue studies of carbonation exist, but there is potential to study the process at Maqarin [204];
- modelling of existing experiments and analogues to better understand the potential significance of uncertainties in predicting the evolution of cement, particularly in the presence of brines. Conventional geochemical models (commonly either the Davies model or the Debye-Hückel model) break down in highly saline conditions; instead, the ‘Pitzer approach’ is commonly used. See the discussion and calculations in Section 6.3.5, which demonstrate the divergence between the Davies and Pitzer approaches for calculating cement evolution in brines over timescales of more than 30 years. Furthermore, there is little evidence with which to predict the long-term evolution of cement in the presence of certain dissolved constituents, most notably high concentrations of Mg;
- further understanding the long-term evolution of different cement formulations. For example, understanding the long-term evolution of low-pH concrete formulations under UK disposal conditions is less well-developed than for Portland cements. A watching brief of the ROMANCON output (see Section 5.2.3.4) could be maintained.

We note that the RWMD Near-field Evolution topic area is already undertaking research into the long-term evolution of cements. The cement-related RDD identified above could be undertaken through the Near-field Evolution area; it would not be appropriate to initiate RDD on cement evolution through the borehole sealing project.

17. Activity 17. Identify advantages and disadvantages of potential materials for the support element for lower permeability sections of borehole: chemical interactions with adjacent clay seals

We recognise an extensive knowledge base already exists on the interactions between clays and other materials. Much of this knowledge comes from research into the behaviour of bentonite buffers around waste canisters, or tunnel backfills. Scaling effects need to be taken into account when applying this knowledge to borehole seals. Compared to these applications, in a borehole seal the area of the interface between the bentonite and adjacent materials will be much larger for a given volume of bentonite. It is necessary to establish whether a given small degree of bentonite alteration or deformation could potentially be more significant for a borehole seal than for a buffer or backfill.

The principal RDD issue is the potential for chemical interaction between cement (a material that potentially could be used in the support, and which is used to cement casings into place) and clay-based seals. Principal research activities are:

- to determine the potential for any development of fractures in and around the clay seal as a result of interactions with cementitious fluids. The presence of smectite minerals in clay seals provides ductility and swelling; such seals would only fracture in the event that reaction with cementitious fluids resulted in significant mineralogical alteration;

- only in the event that the above task indicates the potential for fracturing of the clay seal would further RDD be required to understand how subsequent flow of cementitious fluid through fractures might modify the fracture porosity (e.g. by sealing it or by further opening it). This activity would use the existing knowledge base and coupled transport models to explore the extent and nature of interactions;
- based on the above, understand the potential for alteration to clay seals, the changes to hydraulic properties that could occur and the spatial scales over which changes could occur. If appropriate, propose mitigation measures.

9.3.4 RDD relating to support elements for higher permeability sections of borehole

18. Activity 18. Identify advantages and disadvantages of potential materials for the support element for higher permeability sections of borehole: mechanical stability

- RDD activities should determine the advantages and disadvantages of the potential materials discussed in Section 8.4.2 in terms of mechanical stability and interaction with adjacent seals. As with support elements for lower permeability sections of borehole, the support element for higher permeability sections has no long-term sealing function. However, arguments to support a view on long-term permeability of this support element will need to be developed. These arguments should be based on the existing knowledge base rather on new research activities.
- Loss to the formation should be minimised or controlled when placing the support against highly transmissive structures. A description of material properties required to achieve this should be produced.

19. Activity 19. Identify advantages and disadvantages of potential materials for the support element for higher permeability sections of borehole: chemical interactions with adjacent clay seals

Depending on the materials being considered for support elements in higher permeability sections of borehole, it may be necessary to undertake additional RDD along the lines of Activity 17. As for Activity 17, we recognise an extensive knowledge base already exists on the interactions between clays and other materials.

9.4 RDD relating to the demonstration of seal quality

We propose two activities relating to the demonstration of seal quality.

20. Activity 20. Participation in experiments in overseas Underground Research Laboratories and/or surface sites to build understanding of seal performance and to test QA methodology

Confidence in the performance of borehole seals and supports, or of aspects of them, can be increased through participation in appropriate ongoing experiments in overseas Underground Research Laboratories. Such experiments could provide results on the timescale of the generic RDD programme (i.e. leading up to the start of intrusive investigations at one or more potential sites). Potentially relevant ongoing experiments were described in Section 5.2. Some experiments address sealing of the repository near field (see Section 5.2.2.2); others specifically address sealing of boreholes (see Section 5.2.2.3).

Dismantling or 'over-coring' of these experiments enables the seals to be recovered and examined. This would allow the success of material placement strategies to be determined, and would also provide information on seal properties and on processes that might affect these properties in the longer term. This is particularly important for borehole experiments where, unlike near-field sealing experiments, there can be no subsequent man access to the seal to demonstrate performance.

In addition, there is the potential to participate in future experiments at Underground Research Laboratories and/or at surface locations to demonstrate RWMD's preferred sealing concepts for deep site investigation boreholes. This would include testing of the QA methodology, where this cannot be done by reference to other industries or programmes.

21. Activity 21. Use of industrial and natural analogues

Industrial analogues have the potential to identify processes that are relevant to borehole sealing on the timescale of tens to hundreds of years. As stated above, such RDD is only required where information relevant to borehole sealing cannot be derived from existing industrial analogue studies. Examples would include coring of engineered structures where different materials relevant to borehole sealing are in contact, or over-coring of sealed boreholes to recover and test borehole seals.

Natural analogues are one of the lines of approach to build understanding of the performance of materials in sealed boreholes. A significant knowledge base exists (for example, see Sections 5.2.2.5 and 5.2.3.4). The objective of this task will be to identify natural analogues that are most relevant to borehole sealing, and to make recommendations for further work.

9.5 Summary

A summary of our recommendations is given in Table 9-1. Note that Table 9-1 presents activities, not a workflow. It is possible that several activities under each heading could be undertaken in parallel.

Table 9-1 A summary of the recommendations for the generic RDD programme into sealing deep (>200m) site investigation boreholes

Activity	Description
Stage 1 RDD activities, leading to project Hold Point	
1	Demonstrate the potential range of seal permeabilities required by post-closure assessment for different geological environments and disposal concepts in order to assess the appropriateness of various seal concepts
2	Confirm the functional requirements for the various seal and support elements for the RWMD borehole sealing system and confirm ranges of hydraulic properties for various seal and support concepts at placement and at various times after placement
3	Determine the extent to which knowledge gained from repository sealing and from other industries is transferrable to sealing boreholes at a GDF site
4	Use the existing knowledge base to understand the likely evolution of the Borehole Damage Zone in potentially relevant geological environments after borehole sealing, and the extent to which such movements in the rock mass surrounding a sealed borehole could be beneficial or detrimental to long-term sealing performance

Activity	Description
5	Determine whether RWMD's B1 and B3 illustrative seal concepts (the up-scaled SKB Basic Seal concept and a variant of this approach) are potential solutions for post-closure seals in all relevant HSR and/or LSSR
6	Confirm the extent to which repository perturbations (gas generation and repository resaturation) could affect sealed site investigation boreholes
7	Develop QA methodology to demonstrate the quality of the RWMD sealing system
Hold Point	
Stage 2 RDD activities on individual seal/support elements	
RDD relating to post-closure seals in HSR and LSSR Activities 8 to 10 to be undertaken in parallel if Activity 4 concludes RWMD's illustrative concept is a potential solution. Otherwise, only Activity 10 to be undertaken	
8	Design and demonstrate the performance of an up-scaled SKB Basic Seal concept
9	Develop and demonstrate a robust approach to placing additional bentonite before placing the perforated tube in sections of borehole where the casing has locally been milled out
10	Develop a complementary or alternative sealing concept for post-closure seals in HSR and/or LSSR. Priority depends on the outcome from Activity 5
11	Further develop understanding of performance of bentonite in borehole seals
12	Further develop understanding of longevity of bentonite in the borehole sealing environment
RDD relating to post-closure seals in evaporites	
13	Identify strategies for protecting seals that are susceptible to dissolution
14	Build understanding of the long-term performance of salt cement
RDD relating to support elements for lower permeability sections of borehole	
15	Establish the permeability/transmissivity boundary between use of support components for lower and higher permeability sections of borehole
16	Identify advantages and disadvantages of potential materials for the support element for lower permeability sections of borehole: mechanical stability
17	Identify advantages and disadvantages of potential materials for the support element for lower permeability sections of borehole: chemical interactions with adjacent clay seals
RDD relating to support elements for higher permeability sections of borehole	
18	Identify advantages and disadvantages of potential materials for the support element for higher permeability sections of borehole: mechanical stability
19	Identify advantages and disadvantages of potential materials for the support element for higher permeability sections of borehole: chemical interactions with adjacent clay seals
RDD relating to the demonstration of seal quality	
20	Participation in experiments in overseas Underground Research Laboratories and/or surface sites to build understanding of seal performance and to test QA methodology
21	Use of industrial and natural analogues

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Appendices

Appendix 1 Additional groundwater flow calculations: methodology and calculated flow resistances

Appendix 2 Geochemical calculations: methodology and results

Appendix 1 Additional groundwater flow calculations: methodology and calculated flow resistances

A1.1 Flows in a transmissive feature around and to/from a borehole seal

A1.1.1 Flows in a transmissive feature around a borehole seal

A simple model is presented below for the effect of a borehole seal, which might have degraded, on the groundwater flow in a transmissive feature. The feature is treated as effectively planar, the flow is represented as two-dimensional (in the plane of the feature) and flow between the feature and the surrounding rocks is neglected. The feature is characterised by its transmissivity, which is taken to be homogeneous and isotropic within the feature. The borehole seal is taken to be a circular region with transmissivity differing from that of the feature. This corresponds to a borehole crossing the feature normal to the feature. The case of steady flow that is uniform at some distance from the borehole is considered.

The x-axis is taken to be along the direction of the flow in the feature at some distance from the borehole. In radial coordinates centred on the axis of the borehole, the equation for groundwater flow in the feature is:

$$\frac{T}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h}{\partial r}\right)+\frac{T}{r^2}\frac{\partial^2 h}{\partial \theta^2}=0$$

where
T is the transmissivity of the feature
h is the groundwater head
r is the radial coordinate
θ is the azimuthal coordinate.

T is the effective transmissivity of the feature. If the feature were a permeable rock formation, then the transmissivity would be given by

$$T = bK$$

where
b is the thickness of the rock formation
K is the hydraulic conductivity of the rock formation.

The equation for flow within the borehole seal is a similar equation with the transmissivity T replaced by the transmissivity of the seal in the plane of the feature T_s. At the boundary between the seal and the feature, the boundary conditions are that the head should be continuous and that the normal component of the flow $-T\frac{\partial h}{\partial r}$ should be continuous.

Using the method of separation of variables, it is easy to show that functions of the form:

$$(C_n \cos n\theta + D_n \sin n\theta)r^n + (E_n \cos n\theta + F_n \sin n\theta)r^{-n}$$

where C_n, D_n, E_n and F_n are constants, satisfy the flow equation.

At large distances from the borehole (relative to its radius), the flow corresponds to a uniform head gradient, that is to:

$$h = Gx = Gr\cos\theta$$

where $-G$ is the head gradient in the x direction at large distances from the borehole.

The boundary conditions do not couple different angular modes. It is therefore appropriate to seek a solution to the flow equations that only involves terms in $\cos\theta$. Thus a solution is sought of the form

$$h = Ar\cos\theta + B\cos\theta / r$$

outside the borehole, and

$$h_s = A_s r\cos\theta + B_s \cos\theta / r$$

inside the borehole. In order to match the conditions at large distances from the borehole

$$A = -G$$

The second term in the expression for h_s is singular at the origin, which is unphysical, and so:

$$B_s = 0$$

The solution for the flow in the whole domain is obtained by combining the two expressions in their appropriate domains together with the conditions that the head and normal component of flow at the borehole surface are continuous.

Continuity of head at the borehole surface ($r = a$, where $r = a$ is the borehole radius) gives:

$$A_s a\cos\theta = -Ga\cos\theta + B\cos\theta / a$$

Continuity of the normal component of flow at the borehole surface gives:

$$-T_s(A_s\cos\theta) = -T(-G\cos\theta - B\cos\theta / a^2)$$

It can be seen that, in both the equations above, the angular dependence of all the terms is the same and so, provided that the equations hold for one value of the azimuthal angle, they hold for all values.

It is straightforward to solve these equations to obtain:

$$B = -\frac{(T - T_b)}{(T + T_b)}Ga^2$$

$$A_s = -\frac{2T}{(T + T_s)}G$$

The total flow through the seal is then given by:

$$Q = -2aT_sA_s = -\frac{2TT_s}{(T+T_s)}Ga$$

From the results above, it can be readily seen that the flow is only perturbed within a distance from the borehole of the order of the borehole radius. If the seal has much lower transmissivity than the feature, then the total flow through the seal is greatly reduced from the flow $Q = -2aTG$ that would otherwise occur. The flow that would have passed through the region where the seal is present is diverted around the seal. Conversely, if the seal has degraded to the point where it is much more transmissive than the feature, then the flow in the vicinity of the borehole is focused into the feature, leading to a total flow through the seal that is approximately twice the flow that would occur through the region occupied by the seal were it not present.

The model described above is an idealisation. Nevertheless, it represents the main feature of the system of interest. The model could be extended to take into account, for example, the presence of a disturbed zone around the borehole or a borehole that crosses the transmissive feature at an angle. However, the analysis becomes more complicated, and it would probably be better to carry out the calculations using suitable numerical models.

A1.1.2 Flows in a transmissive feature to/from a borehole

A simple model is presented below for the flow in a transmissive feature to or from a borehole in the case in which the borehole seals have degraded to the extent that there can be significant flow along the borehole. Assumptions regarding geometry and flow within the transmissive feature and borehole are as in the previous Section. The case of steady radial flow to the borehole is considered. As previously, this is an idealisation and a more detailed analysis could be undertaken using suitable numerical models.

The case in which, at a distance from the borehole, there is a background flow in some direction, can be handled to a very good approximation by combining the model discussed in the previous Section with the model presented in this Section. This is because of the linearity of the governing flow equation.

The equation for radial flow in the feature is:

$$\frac{T}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h}{\partial r}\right) = 0$$

The steady-state solution to this equation, which can be readily derived, is:

$$h = A + B\ln(r)$$

Where A and B are constants.

If the head is h_a at the surface of the borehole (at radius a) and the head is h_R at some large distance R from the borehole, then:

$$B = \frac{(h_R - h_a)}{\ln(R/a)}$$

$$A = \frac{(h_a \ln(R) - h_R \ln(a))}{\ln(R/a)}$$

The flow to the borehole is given by:

$$Q = 2\pi BT = \frac{2\pi T(h_R - h_a)}{\ln(R/a)}$$

This can be expressed as:

$$Q = \frac{(h_R - h_a)}{R_{HF}}$$

Where:

$$R_{HF} = \frac{\ln(R/a)}{2\pi T}$$

is a flow resistance.

In the above, R is effectively the distance at which the head in the feature is controlled by the groundwater flow in the surrounding rocks. In practice, this distance is likely to be of the order of hundreds of metres. It should be noted that the flow is not very sensitive to the value of R for values of the order expected. For example, the flow for R=1,000m is only 25% less than the flow for R=100m.

It is worth considering the transient development to the steady-state solution discussed. If the head in the feature is initially h_R everywhere and the head at the borehole is suddenly changed to h_a, then a region around the borehole in which the change in head is proportional to $\ln(r)$ develops and grows with time t like $\sqrt{Dt}$ where $\sqrt{Dt}$ is the hydraulic diffusivity, which is given by:

$$D = T/S$$

where S is the storativity of the feature.

In practice, the time for the steady-state solution to be approached will be very small compared to the times of interest.

A1.2 Flow along a borehole

For each section of sealed borehole, three potential paths for flow can be identified (see Figure 6-2):

- Flow along a degraded seal
- Flow along the boundary between the seal and the surrounding rock

- Flow in a possible damaged zone of rock immediately surrounding the borehole

In addition, we consider flow through the undisturbed rock surrounding the borehole.

Simple models are presented below.

A1.2.1 Flow along a degraded seal

In this case, the total flow is given by:

$$Q = \pi a^2 K \frac{(h_1 - h_2)}{l}$$

where
a is the radius of the borehole
K is the hydraulic conductivity of the degraded seal
l is the length of the section
h_1, h_2 are the heads at the ends of the section.

This can also be written as:

$$Q = \frac{(h_1 - h_2)}{R_{HS}}$$

Where:

$$R_{HS} = \frac{l}{\pi a^2 K}$$

is the flow resistance.

A1.2.2 Flow along the boundary between the seal and the surrounding rock

In this case, the total flow is given by:

$$Q = 2\pi a T_B \frac{(h_1 - h_2)}{l}$$

where T_B is an effective transmissivity for the boundary between the seal and the surrounding rock

This can also be written as:

$$Q = \frac{(h_1 - h_2)}{R_{HB}}$$

Where:

$$R_{HB} = \frac{l}{2\pi a T_B}$$

is the flow resistance.

A1.2.3 Flow in the damaged zone

In this case, the total flow is given by:

$$Q = 2\pi(a + \tfrac{1}{2}\Delta)\Delta K_{DZ}\frac{(h_1 - h_2)}{l}$$

Where:

Δ is thickness of the damaged zone

K_{DZ} is the effective hydraulic conductivity of the damaged zone in the direction along the borehole.

This can also be written as:

$$Q = \frac{(h_1 - h_2)}{R_{HDZ}}$$

Where:

$$R_{HDZ} = \frac{l}{2\pi(a + \tfrac{1}{2}\Delta)\Delta K_{DZ}}$$

is the flow resistance.

A1.2.4 Flow in the background rock surrounding the borehole

The case of interest is that shown in Figure 6-3. Flow is considered along three sections of borehole. In the upper and lower sections, flow occurs in all four potential flow paths: the degraded seal, the boundary between the seal and the surrounding rock, the damaged zone and the background rock. For convenience, these sections are referred to hereafter as ‘flowing sections’. The flowing sections are separated by a section where the seal has not degraded significantly and there is little flow along the seal, the boundary between the seal and the surrounding rock or the damaged zone. In this central section, as shown in Figure 6-3, the flow is through the background rock surrounding the borehole. Such flow is not one-dimensional, and it is not as easy to develop a simple model for the flow as it was for the previous three cases. Numerical modelling would be required to develop a very accurate model for the flow.

However, a reasonable representation that is considered to capture the main features of the flow can be developed as follows. The flow is approximated as the combined flow of a point source near the end of one of the flowing sections and a point sink near the end of the other flowing section as shown in Figure A1-1. Assuming that the damaged zones of the flowing sections carry significant flow, the point sink and source are taken to be a distance a_{DZ} from the ends of the flowing section, as shown in Figure A1-1, where is the outer radius of the damaged zone. So:

$$a_{DZ} = a + \Delta$$

The magnitude of the point sink and source are chosen so that the head at a distance a_{DZ} from the point sink is approximately h_2 and the head at a distance a_{DZ} from the point source is h_1. (If the damaged zones do not carry significant flow then the analysis would be slightly modified. The point sink and source would be taken to be at a distance a from the ends of the flowing sections, and the magnitudes of the point sink and source would be chosen so that the heads at a distance a from the point sink and source are h_2 and h_1 respectively.)

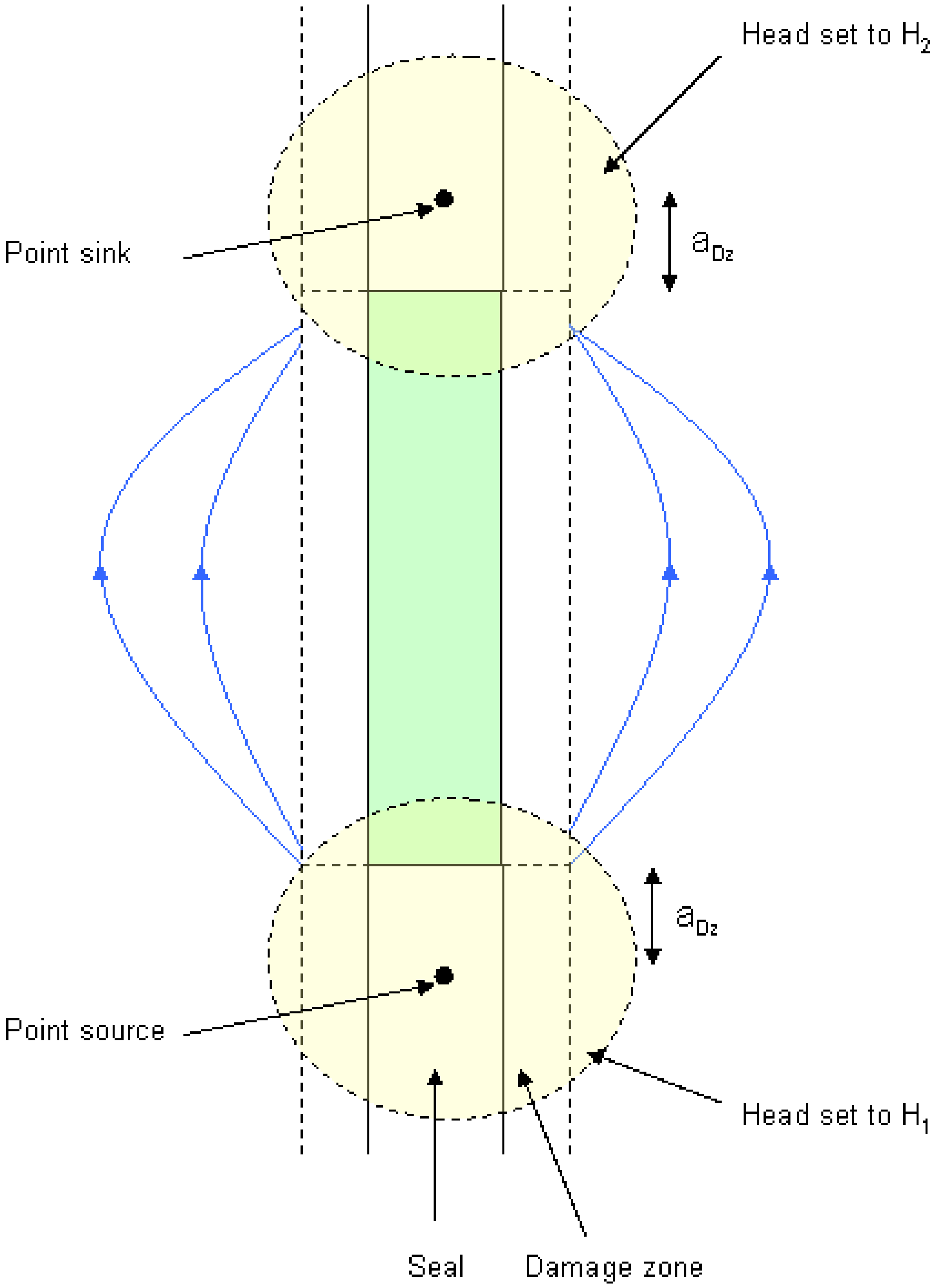


Figure A1-1 Modelling the flow in the background rock between two flowing sections in terms of a point sink and a point source

For a point sink (or source) in an infinite medium, the flow field is spherically symmetric, and the flow equation in spherical coordinates centred on the sink (source) is:

$$\frac{K}{\omega^2}\frac{\partial}{\partial r}\left(\omega^2\frac{\partial h}{\partial r}\right)=0$$

where is the radius in the spherical coordinates.

The solution to this equation is:

$$h=\frac{A}{\omega}+B$$

where A and B are constants.

In the case of interest, the head is therefore approximated as:

$$h=\tfrac{1}{2}(h_1+h_2)+\tfrac{1}{2}(h_1-h_2)\frac{a_{DZ}}{\omega_1}-\tfrac{1}{2}(h_1-h_2)\frac{a_{DZ}}{\omega_2}$$

Where:
ω_1 is the distance of a point from the point source
ω_2 is the distance of a point from the point sink.

(In the vicinity of the point source, the third term above is small and nearly constant; and in the vicinity of the point sink, the second term above is small and nearly constant.)

The flow between the point source and sink is given approximately by:

$$Q=4\pi a_{DZ}^2 K\,\tfrac{1}{2}(h_1-h_2)\frac{a_{DZ}}{a_{DZ}^2}=2\pi K a_{DZ}(h_1-h_2)$$

This can also be written as:

$$Q=\frac{(h_1-h_2)}{R_{HR}}$$

Where:

$$R_{HR}=\frac{1}{2\pi a_{DZ}K_{DZ}}$$

is the flow resistance.

Various approximations are made in the simple analysis presented above. Perhaps the biggest approximation is that the effect of the sealed boreholes between the flowing sections is not taken into account. In the case of primary interest, flow would be effectively excluded from this section. There would very little effect away from the ends of the flowing sections. Even near the end of a flowing section, the flow would only be excluded from about 15% of the region around a point sink (or source). The approximation is therefore considered to be acceptable.

In this approximation, flow resistance does not depend on the length of the section. At first sight, this might seem strange. However, it can be understood as follows. If the separation of the flowing sections is increased, then the flow through the background rock spreads out to cover a bigger region. The dominant contribution to the flow resistance does not come from that part of the domain where the flow is over a long distance and spread out over a large region, but from the small regions near the ends of the flowing sections where the flow is spreading out from regions with dimensions of order aZ.

A1.3 Overall flow along a borehole

In a particular case of interest, a simple model for the overall flow along a borehole can be obtained by combining appropriately the models described above. The flow resistances for the different flow paths along a borehole section are effectively in parallel. The overall flow resistance for the section (R_H) is therefore given by:

$$\frac{1}{R_H} = \frac{1}{R_{HS}} + \frac{1}{R_{HB}} + \frac{1}{R_{HDZ}} + \frac{1}{R_{HR}}$$

where:
R_{HS} is the flow resistance of the seal
R_{HB} is the flow resistance of the interface between seal and rock
R_{HDZ} is the flow resistance of the BDZ
R_{HR} is the flow resistance of the undisturbed rock

The overall flow resistance for the section is therefore largely determined by the smallest of the flow resistances for the different paths.

The overall flow resistances for different sections of boreholes and for the flow to/from a transmissive feature are effectively in series, and so the flow resistances add. The overall flow resistance is therefore largely determined by the largest of the individual resistances.

A1.4 Calculations of flow resistance

The overall flow resistance corresponding to particular combinations of the different resistances can readily be obtained by combining appropriately the different resistances. In most cases, it is sufficient simply to identify the controlling flow resistance.

For definiteness, the radius of a borehole has been taken to be 0.05m (5 cm), and the thickness of a damaged zone has also been taken to be 0.05m. The latter is considered to be a reasonable value on the basis that stress change resulting from the construction of a borehole would largely fall off over such a distance. However, in some circumstances there could be damage over a larger region as a result of borehole construction. For definiteness, the length of the borehole section is taken to be 200m.

In Table A1-1, values of the flow resistance for flow in a transmissive feature to/from a borehole are presented for different values of the transmissivity of the feature. It is considered that a transmissivity up to 10^{-5} m^2s^{-1} would be a possible value (see Table 3-1), which could, for example, correspond to a 1m thick feature with an effective hydraulic conductivity of 10^{-5} ms^{-1}, but a wide range of values are also possible. The radius R is taken to be 100m. (As noted in Appendix 1.1.2, the flow resistance is not very sensitive to the value of R.)

Table A1-1 Values of the flow resistance for flow to/from a borehole in a transmissive feature

Transmissivity [m^2s^{-1}]	Flow resistance [$s.m^{-2}$]
1.0 E-10	1.1 E+10
1.0 E-09	1.1 E+09
1.0 E-08	1.1 E+08
1.0 E-07	1.1 E+07
1.0 E-06	1.1 E+06
1.0 E-05	1.1 E+05

Flow resistances for the various flowpaths along the borehole are calculated in Table A1-2 to Table A1-5. In these tables, the flow for a head difference of 50m is also presented.

In Table A1-2, values of the flow resistance for a borehole seal are presented for different values of the effective hydraulic conductivity in the direction along the seal. SKB calculations show their reference design seal (the basis of the B1 sealing concept) will achieve a hydraulic conductivity of 10^{-12} ms^{-1}. In consequence, we consider a wide range of hydraulic conductivity (from 10^{-14} ms^{-1} to 10^{-5} ms^{-1}) to simulate intact and degraded seals. For definiteness, the length of the borehole section was taken to be 200m.

Table A1-2 Values of the flow resistance for a borehole seal. A wide range of hydraulic conductivities is presented to reflect both intact and degraded seals

Hydraulic conductivity [ms^{-1}]	Flow resistance [$s.m^{-2}$]
1.0 E-14	2.6 E+18
1.0 E-13	2.6 E+17
1.0 E-12	2.6 E+16
1.0 E-11	2.6 E+15
1.0 E-10	2.6 E+14
1.0 E-09	2.6 E+13
1.0 E-08	2.6 E+12
1.0 E-07	2.6 E+11
1.0 E-06	2.6 E+10
1.0 E-05	2.6 E+09

In Table A1-3, values of the flow resistance for the interface between the seal and the rock are presented for different values of the effective aperture at the interface. The transmissivity of the interface is given by:

$$T = \frac{10^7 e^3}{12} \text{ [m}^3\text{]}$$

where e is the aperture [m]. The values presented in this table highlight the importance of ensuring a good contact between the seal and the rock. (Otherwise, the flow resistance is very low.) For definiteness, the length of the borehole section was taken to be 200m.

Table A1-3 Values of the flow resistance for the interface between seal and rock

Effective aperture [micron]	Flow resistance [s.m^{-2}]
1	7.6 E+14
3.1	2.6 E+13
10	7.6 E+11
31	2.6 E+10
100	7.6 E+08
310	2.6 E+07
1000	7.6 E+06

In Table A1-4, values of the flow resistance for the damage zone are presented for different values of the effective hydraulic conductivity in the direction along the borehole. In Table 3-1, hydraulic conductivity of LSSR is given in the range 10^{-10} to 10^{-13} ms^{-1}, whilst the range for HSR the scales of tens of metres is given as 10^{-9} to 10^{-13} ms^{-1}. Values of the flow resistance are presented for a range of larger values of the effective hydraulic conductivity, representing the effects of a higher host rock hydraulic conductivity and some borehole-related damage. For definiteness, the length of the borehole section was taken to be 200m.

Table A1-4 Values of the flow resistance for the borehole damaged zone

Hydraulic conductivity [ms^{-1}]	Flow resistance [s.m^{-2}]
1.0E-13	8.5 E+16
1.0E-12	8.5 E+15
1.0E-11	8.5 E+14
1.0E-10	8.5 E+13
1.0E-09	8.5 E+12
1.0E-08	8.5 E+11
1.0E-07	8.5 E+10
1.0E-06	8.5 E+09
1.0E-05	8.5 E+08

In Table A1-5, values of the flow resistance for the background rock are presented for a large range of effective hydraulic conductivity, based on the information presented in Table 3-1.

Table A1-5 Values of the flow resistance for the undisturbed rock

Hydraulic conductivity [ms^{-1}]	Flow resistance [$s.m^{-2}$]
1.0 E-13	1.6E+12
1.0 E-12	1.6E+11
1.0 E-11	1.6E+10
1.0 E-10	1.6E+09
1.0 E-09	1.6E+08
1.0 E-08	1.6E+07

Appendix 2 Geochemical calculations: methodology and results

A2.1 Bentonite-based seals

A2.1.1 Composition of bentonite and waters

Some simple scoping simulations were carried out to illustrate coupled chemical / transport processes within a bentonite-based seal, for a bentonite composition shown in Table A2.1. The simulated borehole geometry is described in Section 6.3 and illustrated in Figure 6-4.

Table A2.1 Simplified bentonite composition used in the simulations

Component	Units	Value
Porosity	%	30
Montmorillonite	Wt%	75
Quartz	Wt%	22.5
Carbonate (calcite)	Wt%	1.5
Pyrite	Wt%	0.5
Gypsum	Wt%	0.5

The simplified bentonite composition contains 75wt% montmorillonite, which is the minimum amount specified for bentonite buffer material by SKB [205]. The porosity of 30% was specified to be consistent with the grain density of 2,750 kg/m^3 and a dry density of a B1 seal of 1,900 kg/m^3 (Section 2.5.2).

The initial porewater in the bentonite and the host rock porewater compositions, which are applied at the outer boundary of the model, are given in Table A2-2. It should be noted that the fixed water composition on the model boundary will tend to result in seal alteration rates being overestimated in circumstances where mass transport through the surrounding rock is dominantly by diffusion.

Table A2.2 Water compositions used in the simulations

Determinand	Units	Bentonite Porewater	Saline Water (2) (Table 3-3)	Ca-Na-HCO_3 fresh water (3) (Table 3-3)
			Based on [27]	Based on [27]
pH		6.45	7.5	7.5
Na	Mol/kg	1.17E-01	2.86E-01	5.65E-04
K	Mol/kg	4.04E-04	2.61E-03	5.11E-05
Mg	Mol/kg	1.31E-03	4.98E-03	4.53E-04
Ca	Mol/kg	2.77E-03	2.06E-02	8.23E-04
Cl	Mol/kg	1.13E-01	3.22E-01	3.38E-04
SO_4	Mol/kg	4.79E-03	9.25E-03	9.37E-05
HCO_3	Mol/kg	Calcite equilibrium	4.92E-04	2.03E-03
SiO_2	Mol/kg	3.92E-04	Chalcedony equilibrium	Chalcedony equilibrium
AlO_2^-	Mol/kg	1e-16	1e-16	1e-16

The simulations allowed the secondary alteration products given in Table A2.3 to form in the event that they were calculated to become thermodynamically stable.

Table A2.3 Potential bentonite alteration products (compositions from Geochemists Workbench database thermo.com.v8.r6+ [194])

Na-Saponite	$Na_{0.33}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$
K-Saponite	$K_{0.33}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$
Ca-Saponite	$Ca_{0.165}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$
Mg-Saponite	$Mg_{0.165}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$
Na-Beidellite	$Na_{0.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2$
K-Beidellite	$K_{0.33}Al_{2.33}Si_{3.67}O_{10}(OH)_2$
Ca-Beidellite	$Ca_{0.165}Al_{2.33}Si_{3.67}O_{10}(OH)_2$
Mg-Beidellite	$Mg_{0.165}Al_{2.33}Si_{3.67}O_{10}(OH)_2$
Kaolinite	$Al_2Si_2O_5(OH)_4$
Analcime	$Na_{0.96}Al_{0.96}Si_{2.04}O_6 \cdot H_2O$
Illite	$K_{0.6}Mg_{0.25}Al_{1.8}Al_{0.5}Si_{3.5}O_{10}(OH)_2$
Chalcedony	SiO_2
Gypsum (also a primary phase)	$CaSO_4 \cdot 2H_2O$
Anhydrite	$CaSO_4$
Dolomite	$CaMg(CO_3)_2$

A2.1.2 Treatment of kinetics

The simulations represented the kinetics of mineral dissolution / precipitation reactions, using a Transition State Theory (TST)-based approach represented by [206] and [207] *inter alia*):

$$\frac{dS}{dt} = A(S)(k_1 a_H^{n1} + k_2 + k_3 a_H^{n3} + k_4 f_{CO2}^{n4})(Q/K - 1)$$

where S (mol) is the abundance of the solid of interest, t is time (s), $k_{1,2,3,4}$ are the rate constants (mol/(m^2 s)) for acid, neutral, base and carbonate mechanisms, $A(S)$ is the mineral reactive surface area (m^2) (which depends on the mineral abundance), n is a dimensionless catalysis constant for acid (n_1), base (n_3) and carbonate (n_4) – dependent rates, Q is the ion activity product, a_{H+} is the activity of the hydrogen ion, f_{CO2} is the CO_2 fugacity, and K is the equilibrium constant for mineral dissolution. Except for surface area and k, these terms are dimensionless.

In the model, the effect of temperature on reaction rates is taken into account using the Arrhenius equation, which relates activation energy to reaction rate by:

$$k = Fe^{-\frac{E_a}{RT}}.$$

Here, E_a is the activation energy (J/mol), R is the gas constant (J K^{-1} mol^{-1}), T is the temperature (K) and the pre=exponential factor F is used to fit the expression to a measured rate at a given temperature.

For each mineral in the simulation, values of E_a and values of k_i at 25°C (which will be denoted $k_{i,25}$) are given in Table A2.4. A separate E_a value is given for each pH-dependent mechanism. Therefore each term k_i in the rate equation should be replaced by an Arrhenius equation:

$$k_i = F_i e^{-\frac{E_{a_i}}{RT}}.$$

Table A2.4 Kinetic data

Mineral	Acid		E_a acid	Neutral	E_a neutral	Base		E_a base	Carbonate		E_a carb.
	log $K_{1\ 25°C}$	n_1	kJ/mol	log $K_{2\ 25°C}$	kJ/mol	log $K_{3\ 25°C}$	n_3	kJ/mol	log $K_{4\ 25°C}$	n_4	kJ/mol
	mol/m^2/s^1			Mol/m^2/s^1		mol/m^2/s^1			mol/m^2/s^1		
Illite	-11.72	0.60	46.00	-15.05	14.00	-12.31	-0.60	67.00	-	-	-
Montmorillonites	-12.7	0.35	80.75	-14.54	22.18	-15.66	-0.18	84.94	-	-	-
Saponites	-12.7	0.35	80.75	-14.54	22.18	-15.66	-0.18	84.94	-	-	-
Beidellites	-12.7	0.35	80.75	-14.54	22.18	-15.66	-0.18	84.94	-	-	-
Kaolinite	-11.31	0.78	65.90	-13.18	22.20	-17.05	-0.47	17.90	-	-	-
Analcime	-	-	-			-13.09	-0.36	77.1	-	-	-
Quartz	-	-	-	-13.34	90.10	-	-	-	-	-	-
Chalcedony	-	-	-	-12.77	68.70	-	-	-	-	-	
Calcite	-0.30	1.00	14.40	-5.81	23.50	-	-	-	-3.48	1.00	35.40
Anhydrite	-	-	-	-3.19	14.3	-	-	-	-	-	-
Gypsum	-	-	-	-2.79	14.3*			-	-	-	-
Dolomite	-3.19	0.5	36.1	-7.53	52.2			-	-5.11	0.5	34.8

The simulations for which results are reported in the following Sections were carried out for a temperature of 50 °C.

Data for illite are from [208]. Data for kaolinite, quartz, chalcedony (amorphous silica data were used), calcite, anhydrite, gypsum and dolomite are from [207], data for analcime are from [196]. Montmorillonite rate data were extracted from [209] and [210]. Saponites and beidellites were assumed to react at the same rate as montmorillonite.

Montmorillonite dissolution was modelled using rate data that is fitted to the experimental data on pH-dependence of montmorillonite dissolution rates in [209]. The fit to the data is shown in Figure A2.1. The data were refitted as the rate equation used by [209] is in a slightly different format to that used in the reactive transport models.

There is some evidence to suggest that over the temperature range of concern here, precipitation rates of smectite minerals are approximately an order of magnitude lower than dissolution rates [211]. This assumption is used in the smectite reaction rates in the models described here.

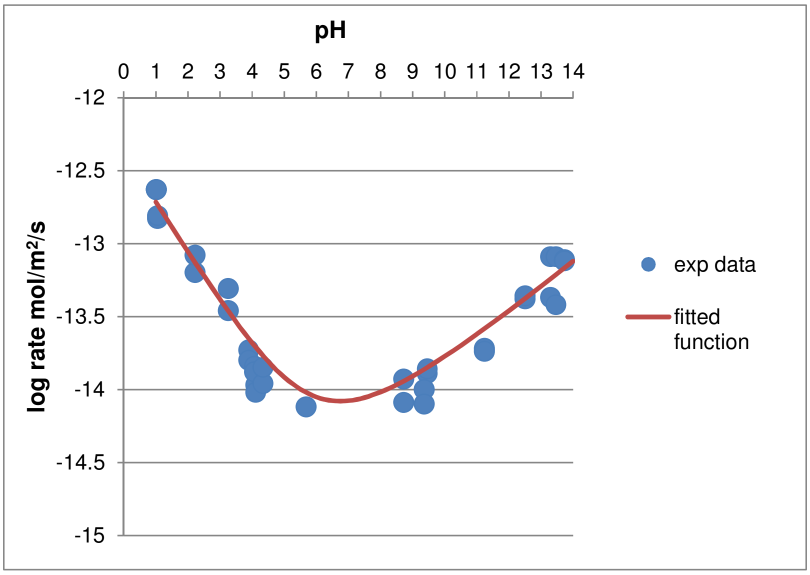


Figure A2.1 Rate of montmorillonite dissolution as a function of pH at 25 °C. Solid line calculated using fitted parameter values, experimental data taken from [209]

Reactive surface area data for minerals were either taken from the literature or were calculated using geometric arguments. See Table A2.5.

Table A2.5 Surface areas of the phases in the simulations

Mineral	Surface Area m^2/g	Notes / References
Illite	130	[208] (reported rate data is BET normalised)
Montmorillonite	111	BET normalised rate data from [209]
Saponite	111	montmorillonite analogue
Beidellite	111	montmorillonite analogue
Kaolinite	8.16	[212] (BET data)
Analcime	0.25	[196] (BET data)
Quartz (alpha)	0.23	geometric calculation: 10 µm sphere
Chalcedony	2.30	geometric calculation: 1 µm sphere
Pyrite	0.12	geometric calculation: 10 µm sphere
Calcite	0.22	geometric calculation: 10 µm sphere
Anhydrite	0.20	geometric calculation: 10 µm sphere
Gypsum	0.26	geometric calculation: 10 µm sphere
Goethite	0.16	geometric calculation: 10 µm sphere
Dolomite	0.21	geometric calculation: 10 µm sphere

A2.1.3 Thermodynamic data

Equilibrium constants for mineral hydrolysis reactions and reactions between basis aqueous species and other aqueous species were taken from the Geochemist's

Workbench [213] database 'thermo.com.v8.r6+. Standard molar volume data were also taken from this database for many of the relevant solid phases. However, for some smectite end-members and illite this database does not contain appropriate volume data. In these cases, the molar volumes shown in Table A2.6 were calculated using the analogue mineral algorithm approach described by [214]. Ion exchange selectivities for MX80 were taken from [215] and are given in Table A2.7.

Table A2.6 Standard molal volume data for clay minerals (calculated using the analogue mineral algorithm [214])

Mineral	Molal V (cm^3/mol)
Montmor-Na	141.377
Montmor-K	149.067
Montmor-Ca	137.259
Montmor-Mg	134.501
Saponite-Na	146.787
Saponite-K	154.477
Saponite-Ca	142.669
Saponite-Mg	139.911
Beidellite-Na	138.618
Beidellite-K	146.308
Beidellite-Ca	134.500
Beidellite-Mg	131.742
Illite	144.879

Table A2.7 Gaines-Thomas Ion exchange selectivities (values for MX80 bentonite from [215])

Ion exchange reaction	Log K
$XNa + K^+ = XK + Na^+$	0.602
$2XNa + Ca^{2+} = XCa + 2Na^+$	0.415
$2XNa + Mg^{2+} = XMg + 2Na^+$	0.342

A2.1.4 Transport data

In the calculations carried out here, transport through the bentonite was specified to occur only by diffusion. An effective diffusion coefficient value of 7.13 x 10-11 m^2s^{-1} was used. This value is the one given by [216] for bentonite buffer blocks with a dry density of 1,760 kg/m^3 at 25 °C (298K) and most likely will over-estimate the actual initial value that is appropriate for a bentonite comprising a B1 seal that is compacted to a dry density of 1,900 kg/m^3.

During the simulations, the effective diffusion coefficient, $D_{e,298}$, varied as a function of the evolving porosity according to:

$$D_{e,298} = \frac{\theta}{\theta_0} D_{e0,298}$$

where θ_0 is the initial porosity, θ is the porosity following reaction.

The effective diffusion coefficient at the temperature T of the calculation, $D_{e,T}$, was calculated from the effective diffusion coefficient at the reference temperature of 298 K using the following relationship between diffusion coefficient and water viscosity:

$$D_{e,T} = \frac{T}{298} \frac{\eta_{298}}{\eta_T}$$

Where η_{298} is the viscosity at 298 K and η_T is the viscosity at the temperature T, which is calculated from:

$$\eta_T = \eta_{20} \exp\left(-ln10 \times \frac{1.37023(T_C - 20) + 8.36 \times 10^{-4}(T_C - 20)^2}{109 + T_C}\right)$$

where η_{20} is viscosity of water at 20 °C, 1.002×10^{-3} Pa s (e.g. [217]) and T_c is the temperature in degrees celsius.

A2.1.5 Calculation results

The calculations showed clearly the effects of cation exchange (Figure A2.2, Figure A2.3). The bentonite approaches cation exchange equilibrium across the entire width of the seal after about 50 years.

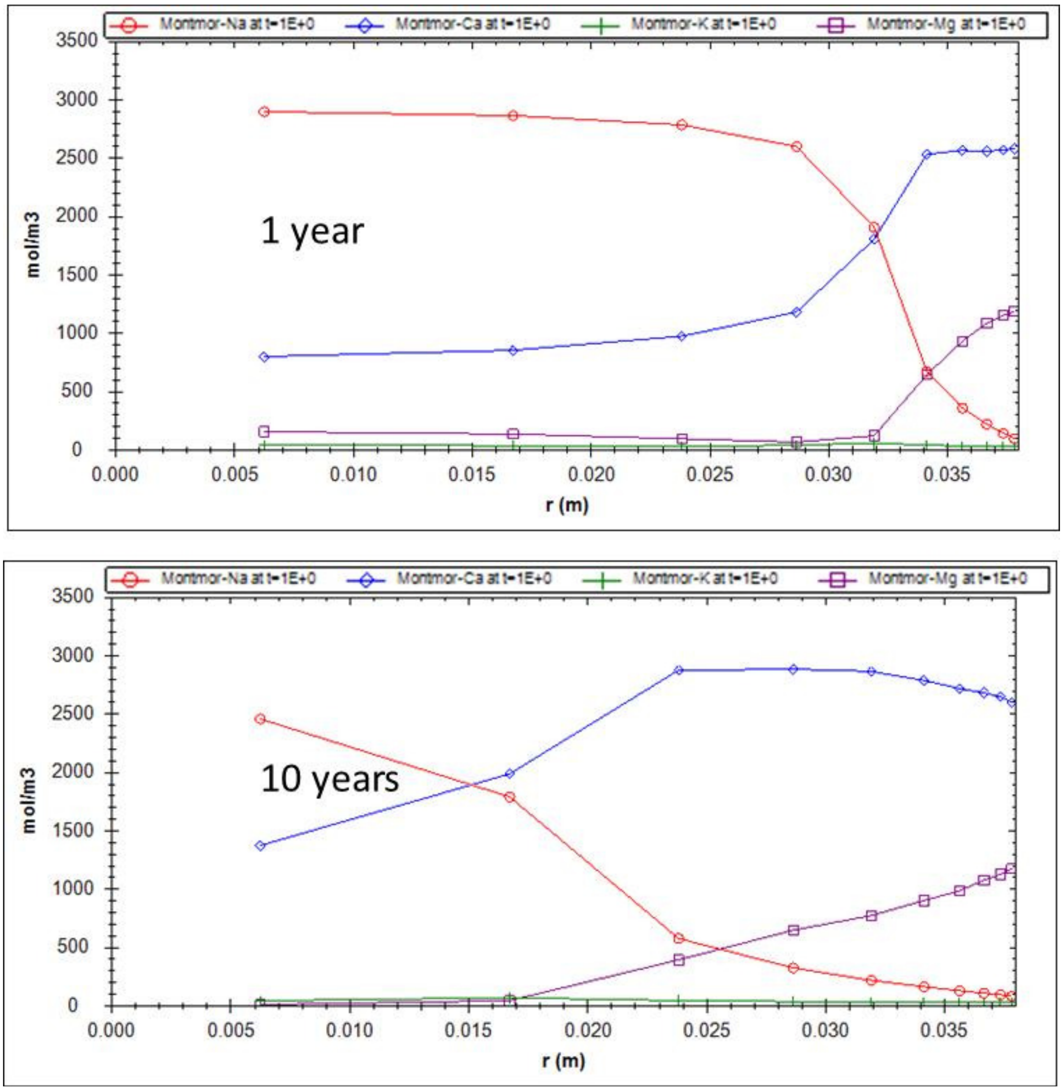


Figure A2.2 Variation in exchangeable cations from the centre (left) to the rim (right) of the bentonite seal, when the groundwater in the surrounding rock is fresh with the composition given in Table A2-2, for a temperature of 50°C

The cation exchange that occurs reflects the composition of the water (Figure A2-3). In the Ca-Na-dominated fresh water, the initially Na-montmorillonite exchanges with Ca and Mg to form Ca-montmorillonite and Mg-montmorillonite respectively, with the former dominating. In contrast, in the saline Na-Cl dominated water the montmorillonite remains Na-exchanged. Corresponding to the ion exchange in the fresh water there would be a reduction in swelling pressure, although this is likely to be small in this case for the dry densities of relevance to borehole seals (e.g. [195]).

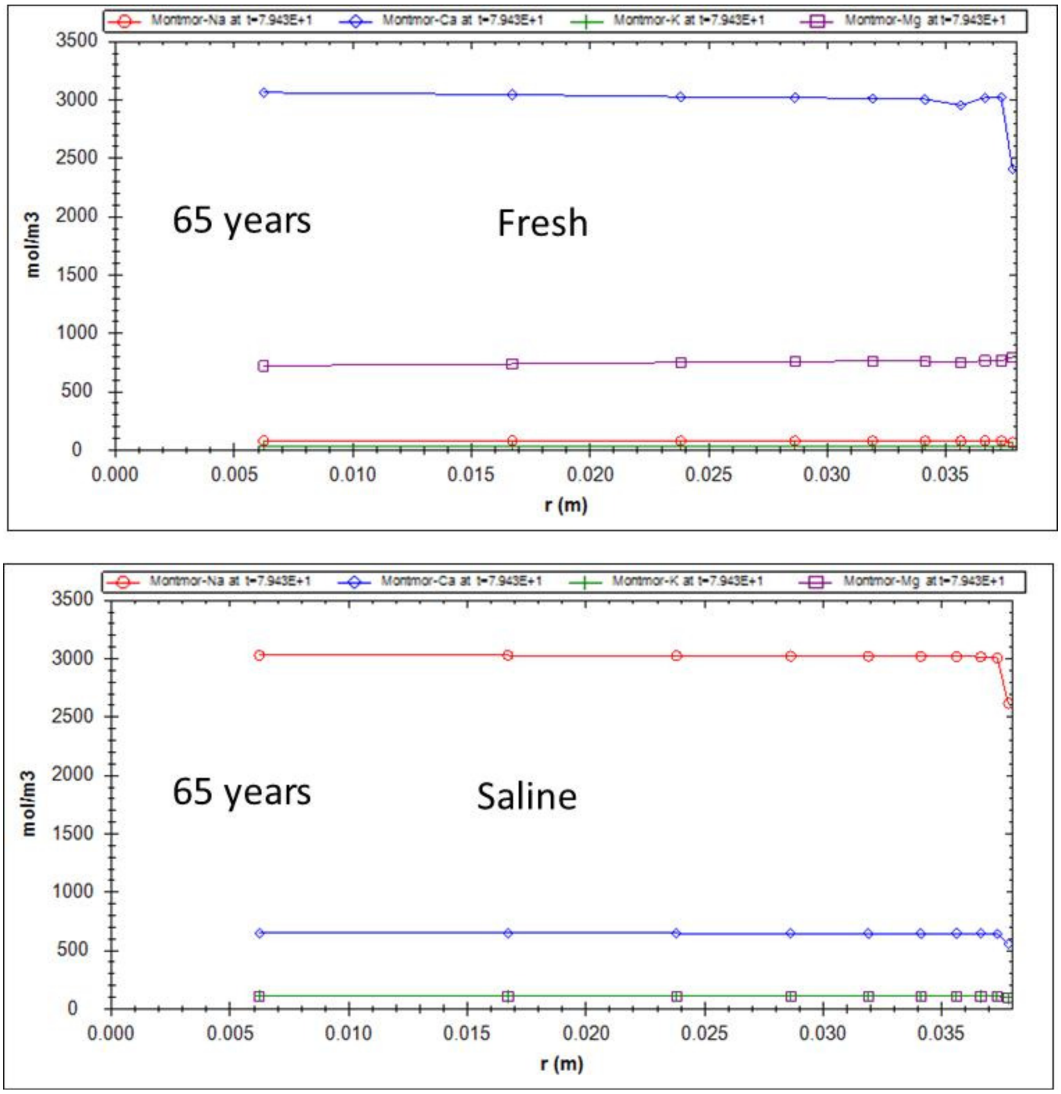


Figure A2.3 Variation in exchangeable cations from the centre (left) to the rim (right) of the bentonite seal2, when the groundwater in the surrounding rock is fresh (above) or saline (below) with the compositions given in Table A2.2, for a temperature of 50 °C.

For simulations with both fresh and saline water compositions (Table A2-2), the porosity of the bentonite was calculated to decrease over time in the vicinity of the outer surface of the seal (Figure A2-4). This reduction in porosity eventually caused mass transport into the bentonite to decrease to the point where chemical changes within the bentonite occurred at an extremely slow rate. This situation occurred after about 80 years in the case of the fresh water and after about 65 years in the case of the saline water.

A result of the slowing rate was that the bulk of the bentonite, more than 1-2 mm from the interface, showed little change in porosity. To some degree the actual timing of pore clogging in this way depends upon the spatial discretization employed by the model; the narrower a compartment the earlier will be the clogging and therefore it is important that the spatial scales that are used are consistent with those that would be expected to be thick enough to provide a genuine barrier to further transport. In the models presented here, the compartment adjacent to the margin of the bentonite was only 0.38 mm thick. However, since the timescales for clogging are very short compared to the timescales over which sealing performance must be maintained, even substantially coarser discretization would give a similar overall result; increasing the thickness of the outer compartment would increase the time required for clogging proportionately, but this time would remain short compared to the timescales over which seal performance is assessed.

In conclusion, the results illustrate that porosity reduction will likely be restricted to the vicinity of seal margin.

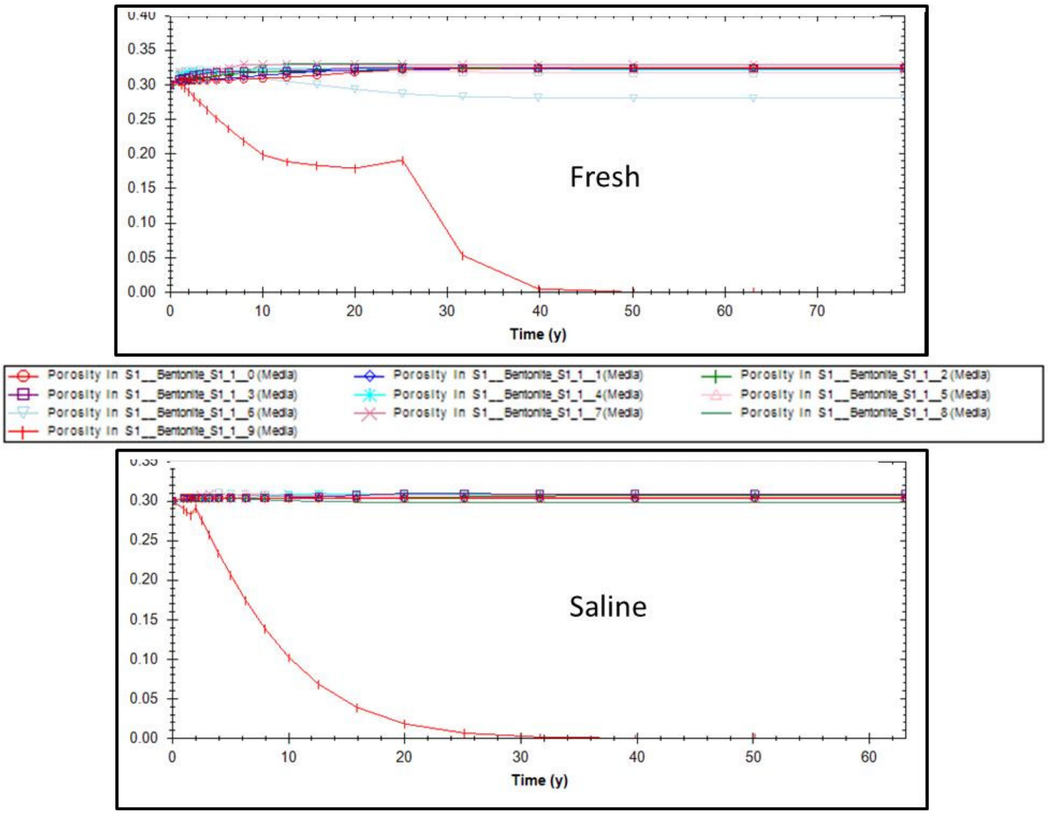
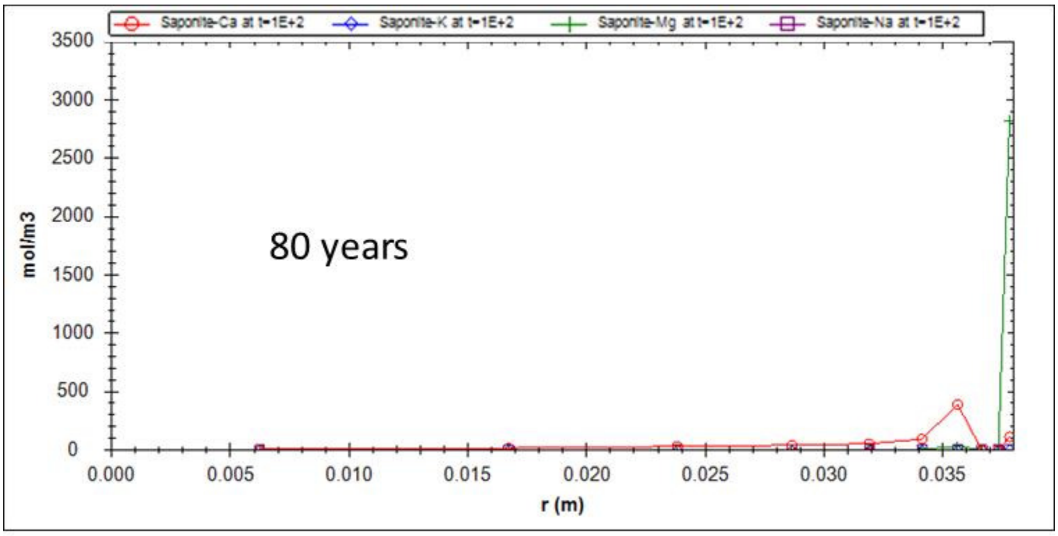


Figure A2.4 Variation in bentonite porosity with respect to time, when the groundwater in the surrounding rock is fresh (above) or saline (below), with the compositions given in Table A2.2 for a temperature of 50 °C. Each curve represents a different compartment in the discretization, with the compartment numbered 0 at the centre of the seal and compartment numbered 9 next to the outer interface.

The cause of the porosity loss near the outer margin of the bentonite was the precipitation of saponite, an Mg-rich smectite clay (Figure A2-5, Figure A2-6). A broadly similar result was given by simulations with both fresh water and saline water, but the composition of the saponite interlayer, where the exchange occurs, differed in each case. The saponite was Mg-dominated in the fresh water case, but Na-dominated in the saline water case. However, this difference is not expected to cause the overall performance of the seal to differ in one case compared to the other. Quite apart from the slowing of mass transport due to the porosity loss in both cases, this reaction is effectively replacing one swelling clay mineral (montmorillonite) by another (saponite).



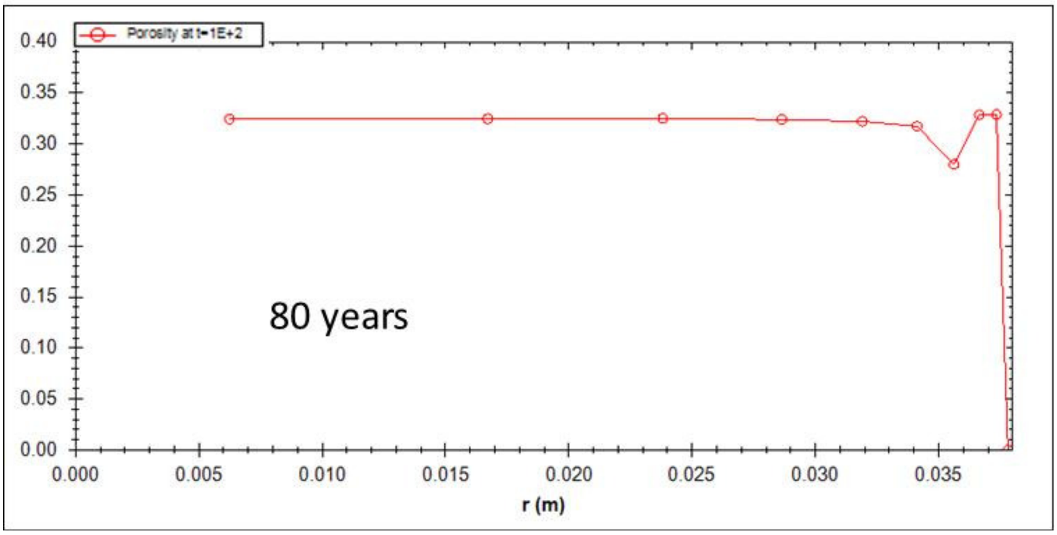


Figure A2.5 Variation in concentration of saponite (above) and porosity (below), between the centre of the bentonite seal (to the left) and the seal margin (to the right), after 80 years in the presence of fresh groundwater with the composition given in Table A2.2, for a temperature of 50 ℃.

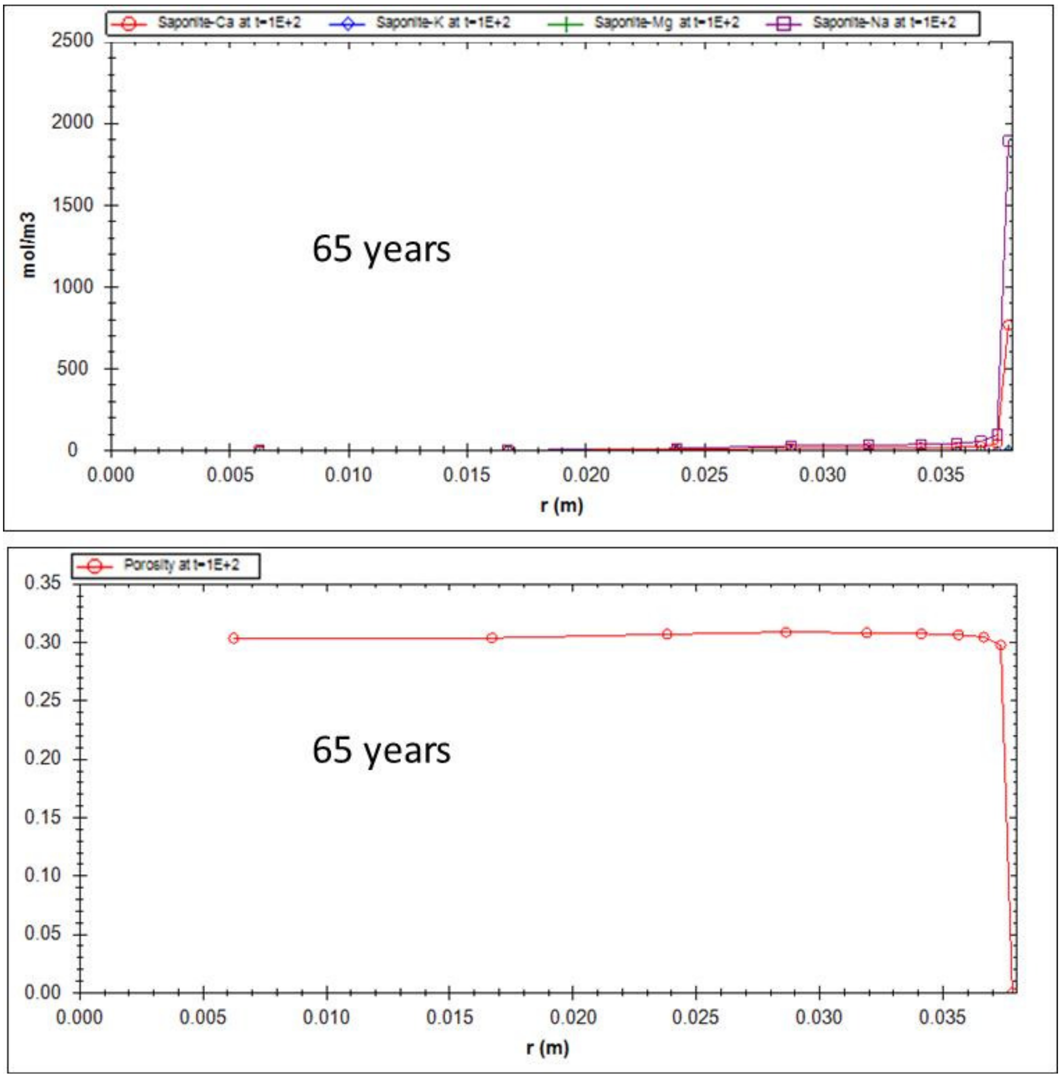


Figure A2.6 Variation in concentration of saponite (above) and porosity (below), between the centre of the bentonite seal (to the left) and the seal margin (to the right), after 65 years in the presence of saline groundwater with the composition given in Table A2.2, for a temperature of 50 °C.

A2.2 Cement-based supports

Illustrative simulations were also undertaken for cementitious (C1) support elements. The basic geometry employed in the simulations was as shown in Figure 6-4. The cement composition was a simplified representation of a Class G cement, which is commonly used in borehole sealing applications (Chapter 4), and is shown in Table A2.8. The porosity was specified to be 30%, consistent with the Class G composition given by [218].

The initial porewater composition in the cement is given in Table A2-9. Simulations used either fresh or saline water, with the compositions given in Table A2-2. It should be noted that the fixed water composition on the model boundary will tend to result in seal alteration rates being overestimated in circumstances where mass transport through the surrounding rock is dominantly by diffusion. However, since cement-based supports will be deployed in higher-permeability rocks, mass transport to the margin of a cement seal will probably be by advection.

Table A2.8 Composition of Class G cement used in the simulations (simplified from [218])

Mineral	Vol/m^3 cement (cm^3)	Mol / m^3
Jennite-07Mat	305,200	3,893
Portlandite	182,700	5,527
Ettringite	96,600	136.6
Katoite	73,500	491.6
Hydrotalcite	37,800	171.7
Calcite	4,200	113.7

Table A2.9 Initial cement porewater composition used in the simulations

Determinand	Units	Initial Cement Porewater	Constraint
pH		13.4	Specified
Na	mol/kg	5.00e-2	Specified
K	mol/kg	1.10E-1	Charge balance
Mg	mol/kg	9.82E-11	Hydrotalcite
Ca	mol/kg	2.72E-3	Portlandite equilibrium
Cl	mol/kg	1.00E-6	Specified
S	mol/kg	5.27E-4	Ettringite equilibrium
C	mol/kg	5.23E-5	Calcite equilibrium
Si	mol/kg	1.07E-4	Jennite equilibrium
Al	mol/kg	1E-16	Monocarbonate equilibrium

A2.2.2 Treatment of kinetics

All minerals were assumed to precipitate or dissolve at a volumetric rate (mol/m^3/s) governed by the following equation (e.g. [219]):

$$\text{rate} = Ak_0\left(a_{H^+}\right)^n(\Omega - 1)$$

Here A_k is the mineral reactive surface area per unit total volume (m^2/g); $k_{0,k}$ is the rate constant at pH = 0 (mol/m^2/s); a_{H+} is the activity of H$^+$ in solution (-); n is a constant (-); and Ω is the ion activity product (IAP) of the mineral divided by the equilibrium constant, K (-). Precipitation occurs if the rate is positive, whereas dissolution occurs when the rate is negative. It should be noted that the above rate law is asymmetric because the range for precipitation is unbounded, whilst dissolution must be in the range [-1, 0] because Ω is always positive.

In the scoping calculations here, for cement minerals the rate constant was specified to be 10^{-12} mol/m$^{/}$s (e.g. [220]). For calcite, a rate constant of $10^{-5.2}$ mol/m$^{/}$s was used. For all minerals, n was set to zero. Following [221], cement minerals were assigned a surface area of 10 m^2/g, apart from calcite which was given a surface area of 0.02 m^2/g.

A2.2.3 Thermodynamic data

There are limited thermodynamic data for the various cement phases over the full temperature range of relevance. For the purposes of the illustrative simulations reported here, thermodynamic data at 15 °C, as given in Table A2-10, were used. The simulations were actually carried out for a temperature of 25 °C, which is a compromise between the need to choose a temperature within the range likely to affect actual seals and the need to ensure that available thermodynamic data are applicable. These data were added to the thermodynamic database "thermo.com.V8.R6". The database "thermo.com.V8.R6" is distributed with the geochemical modelling software Geochemist's Workbench™ (GWB) [213] and is in the format required by CABARET.

The C-S-H gel present within the cement was represented by an ideal solid-solution, based on the model of [222] as redefined by [223] and [224]. In this model a mixture consisting of a tobermorite-like gel (Tob) and a jennite-like gel (Jen) is used to represent CSH with Ca/Si ratios < 1.67. In this case, the mass action equation takes the activity of each end-member in the solid solution to be proportional to its mole fraction, χ i.e.

$$[\mathrm{CSH}_{\mathrm{Jen}}] = \lambda_{\mathrm{Jen}}\ \chi_{\mathrm{Jen}}$$
$$[\mathrm{CSH}_{\mathrm{Tob}}] = \lambda_{\mathrm{Tob}}\ \chi_{\mathrm{Tob}}$$

Here λ is the activity coefficient, which is taken to be unity for an ideal solid solution. Thus:

$$[\mathrm{CSH}_{\mathrm{Jen}}] = \chi_{\mathrm{Jen}} = \frac{m_{\mathrm{Jen}}}{m_{\mathrm{Jen}} + m_{\mathrm{Tob}}}$$
$$[\mathrm{CSH}_{\mathrm{Tob}}] = 1 - \chi_{\mathrm{Jen}}$$

where m_i is the number of moles of the solid solution end member *i*.

The activity model for aqueous species used in this simulation is the Davies Equation (e.g. [225]) which gives the activity coefficient as:

$$\log_{10}(\gamma_i) = \frac{-Az_i^2\sqrt{I}}{1+\sqrt{I}} + 0.2Az_i^2 I$$

where *A* is a constant that varies slightly with temperature, which is again available from compilations of thermodynamic data.

Table A2.10 Thermodynamic data for minerals in the cement at 15 ℃. All data are from [223] except that for calcite which is from HATCHES database. Calcium silicate hydrate phases (CSH) are represented as a solid solution between jennite (Ca/Si = 1.6666) and tobermorite (Ca/Ca = 0.8333)

Mineral	Reaction	$\log_{10} K$
Calcite	$CaCO_3 + H^+ = Ca^{2+} + HCO_3^-$	2.0600
Portlandite	$Ca(OH)_2 + 2H^+ = Ca^{2+} + 2H_2O$	23.5010
CSH (Jennite)	$(CaO)_{1.6666}SiO_2{\cdot}2.1H_2O + 3.3332H^+ = 1.6666Ca^{2+} + SiO_{2(aq)} + 3.7666H_2O$	30.8209
CSH (Tobermorite)	$(CaO)_{0.8333}SiO_2{\cdot}1.3333H_2O + 1.6666H^+ = 0.8333Ca^{2+} + SiO_{2(aq)} + 2.1666H_2O$	11.3534
SiO2am	$SiO_2 = SiO_{2(aq)}$	-2.8080
Ettringite	$Ca_6Al_2(SO_4)_3(OH)_{12}{:}26H_2O + 4H^+ = 6Ca^{2+} + 2Al(OH)_4^- + 3SO_4^{2-} + 30H_2O$	11.3090
Hydrotalcite	$Mg_4Al_2(OH)_{14}{:}3H_2O + 6H^+ = 4Mg^{2+} + 2Al(OH)_4^- + 9H_2O$	29.4140
Monocarbonate	$Ca_4Al_2(CO_3)(OH)_{12}{:}5H_2O + 5H^+ = 4Ca^{2+} + 2Al(OH)_4^- + HCO_3^- + 9H_2O$	35.8310

A2.2.4 Transport data

Variations in the diffusion coefficient as a consequence of evolving porosity were modelled using Archie's Law (e.g. [225])

$$D_e = \frac{D_p}{\theta^{1-m}}$$

where: D_e is the effective diffusion coefficient (m^2/s); D_p is the pore diffusion coefficient (m^2/s); θ is the porosity (-); and m is a constant, which was taken to be 2. Assuming non-porous aggregates and typical OPC parameters, the initial pore diffusion coefficient and porosity of the concrete were set to $3{\times}10^{-11}$ m^2/s.

A2.2.5 Calculation results

For simulations using both fresh water and saline water, the proportion of tobermorite increased relative to jennite towards the margin of the support (Figure A2.7) reflecting the progressive preferential leaching of Ca from the cement at a faster rate than leaching of Si.

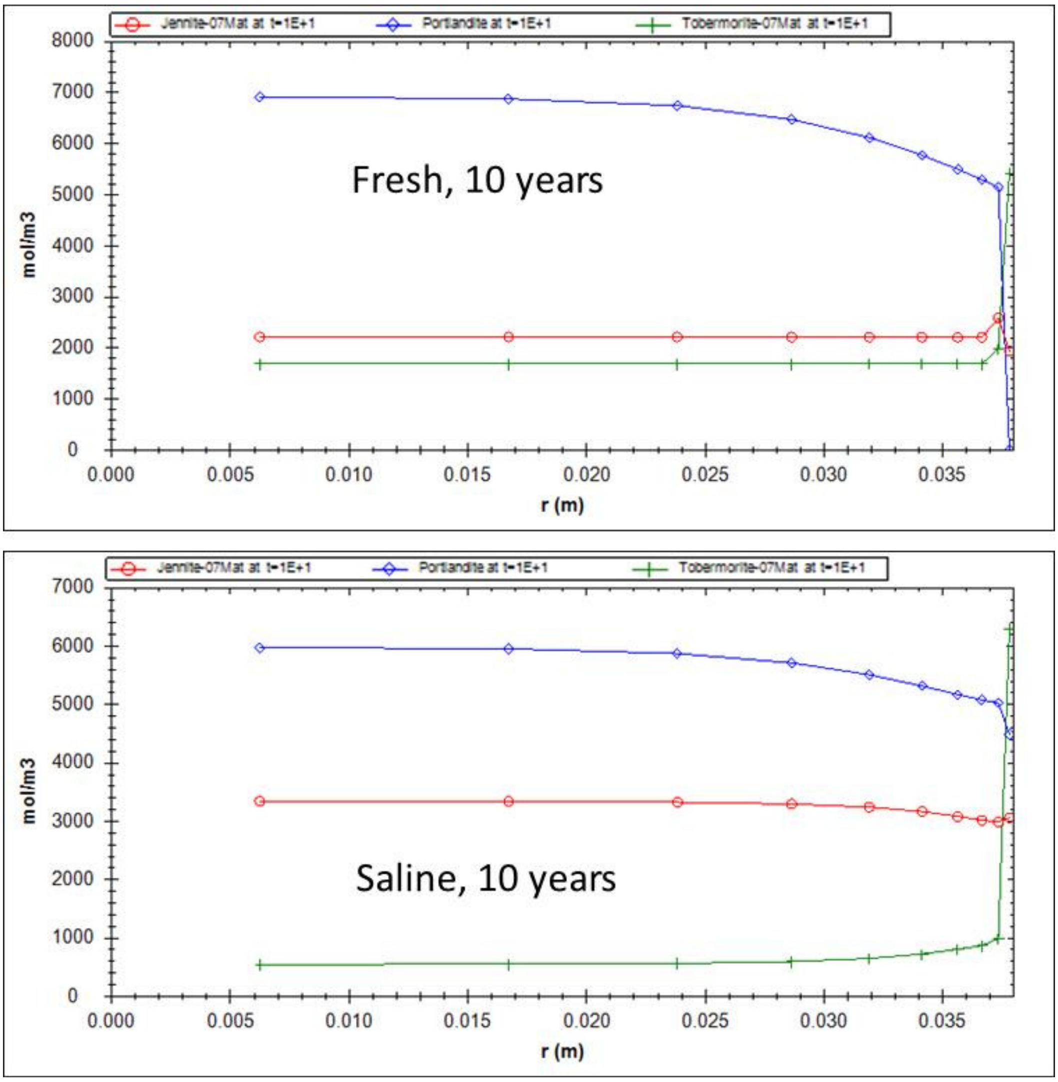


Figure A2.7 Variation in concentrations of jennite-7A (red), tobermorite (green) and portlandite (blue) from the centre of the support (towards the left) to the margin of the support (towards the right) after 10 years in the presence of fresh groundwater (upper) and saline groundwater (lower) with the compositions given in Table A2.2, for a temperature of 50 °C.

These reactions are accompanied by a porosity reduction near the margin (Figure A2-8). However, the porosity throughout the cement increases in the freshwater case, but shows a slight decrease throughout the cement in the saline water case (Figure A2-8). Indeed, the decrease in porosity is such for the saline case that the reactions become extremely slow after about 1,000 years, such that thereafter the properties of the cement change only very slightly.

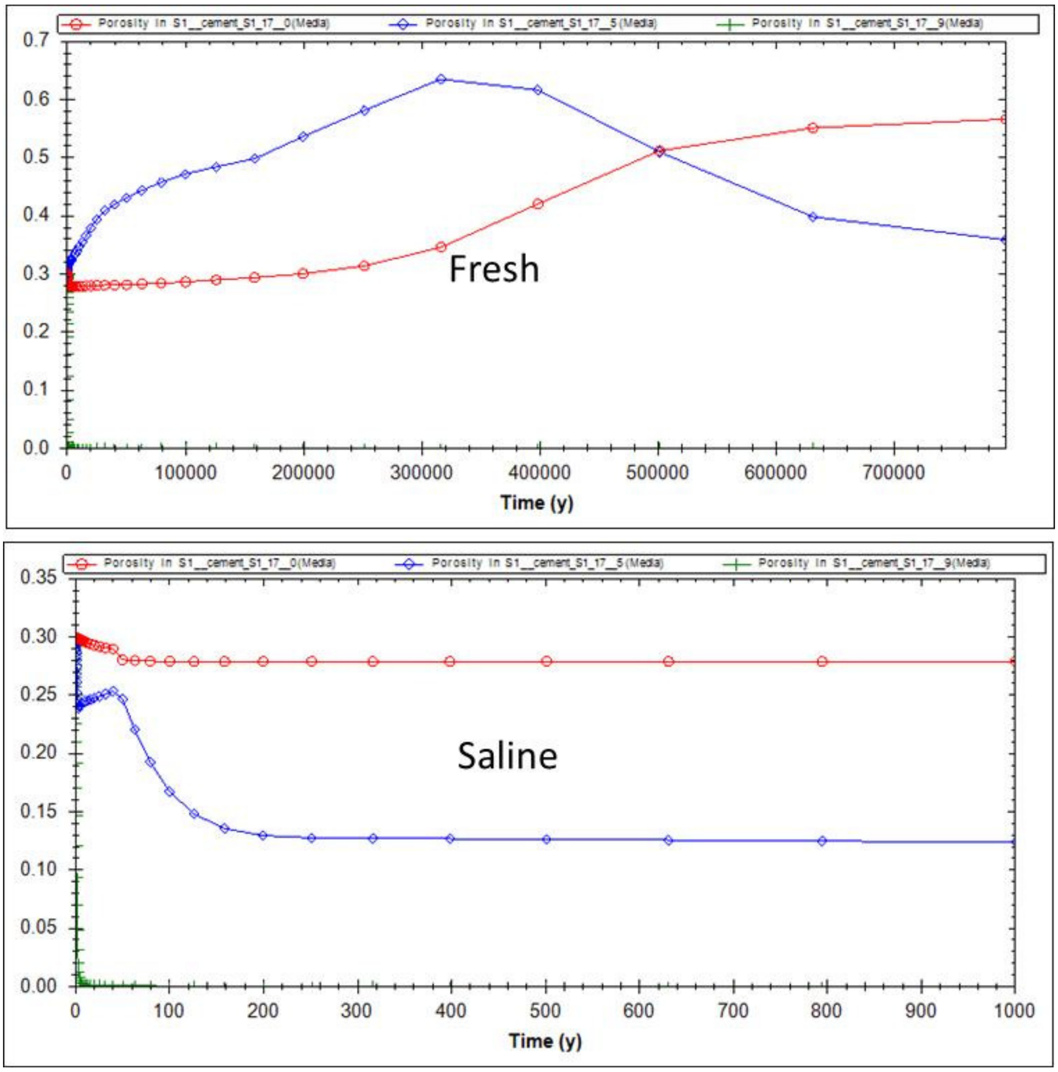


Figure A2.8 Variation in porosity with respect to time for compartment 0 in the centre of the cement support, compartment 5 midway between the centre of the support and the margin, and compartment 9 at the outer margin of the support. The simulations were carried out in the presence of fresh groundwater (upper) and saline groundwater (lower) with the compositions given in Table A2.2, for a temperature of 50 °C.

The porosity reduction at the boundary in both cases was caused by precipitation of calcite (Figure A2.9). In addition, in the saline water case, ettringite also precipitated in a significant quantity, leading to further porosity reduction (Figure A2.9). However, the maximum ettringite precipitation in this case occurred 2 mm into the cement. The precipitation of this phase reflects the penetration of SO_4 into the cement from the surrounding groundwater. The peak in ettringite precipitation does not occur immediately adjacent to the boundary because here the Ca concentration is reduced owing to calcite precipitation.

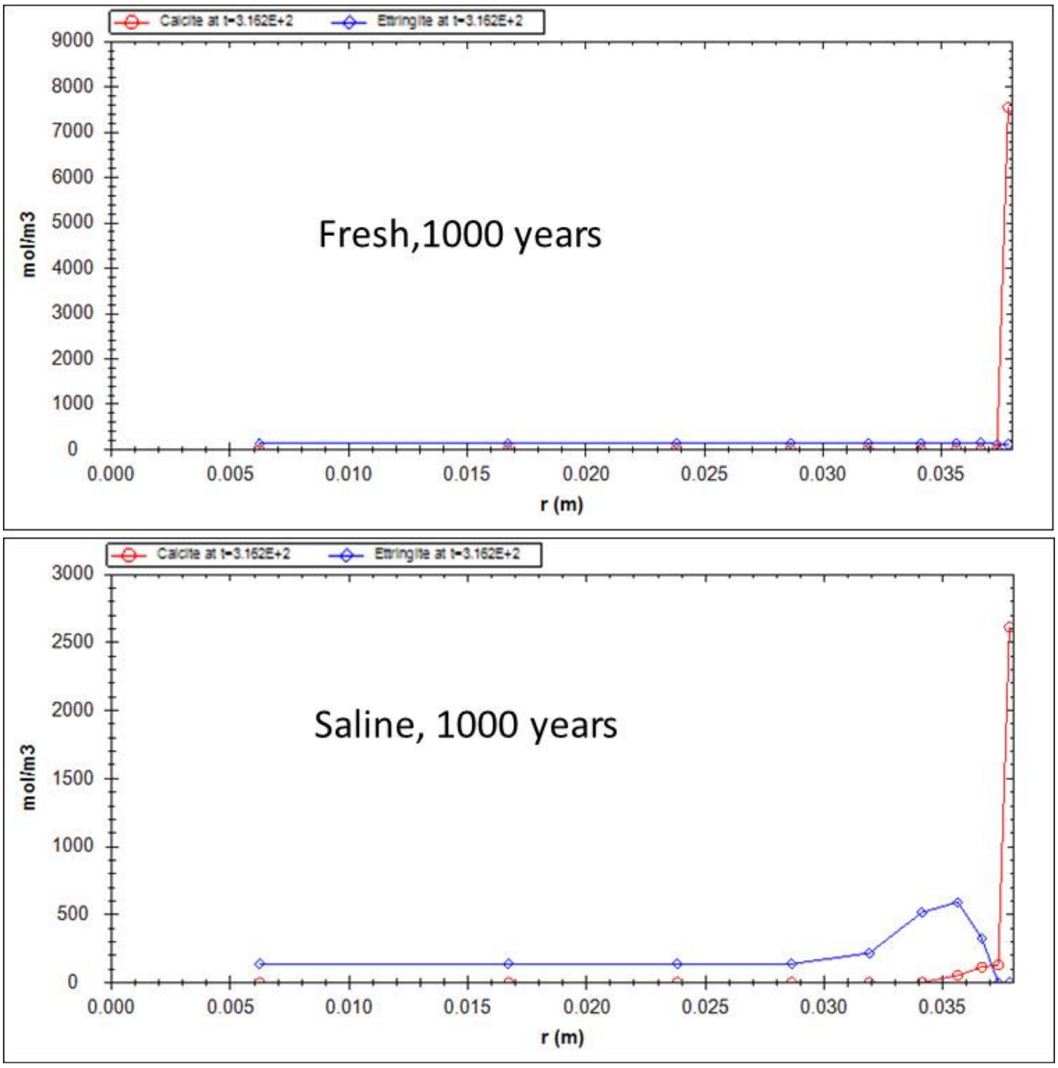


Figure A2.9 Variation in concentrations of calcite (red) and ettringite (blue) from the centre of the support (towards the left) to the margin of the support (towards the right) after 300 years in the presence of fresh groundwater (upper) and saline groundwater (lower) with the compositions given in Table A2.2 for a temperature of 50 °C

A2.3 Cement-bentonite interactions

In the present work cement-bentonite interactions were not investigated by means of new calculations. However, a previous CABARET test case had been constructed to investigate further the cement-bentonite models described by [196]. In these models, a cementitious porefluid of fixed composition is specified to occur at the margin of a bentonite. The bentonite composition is shown in Table A2.11 and the initial porewater compositions are given in Table A2.12. Kinetic, thermodynamic and transport parameters are as given in [196].

Table A2.11 Mineralogical compositions of bentonite and potential secondary minerals in the model based on [196]

Mineral	Formula	Vol.%	mol/m^3
Primary Minerals			
Na-montmorillonite	$Na_{0.33}Mg_{0.33}Al_{1.67}Si_4O_{10}(OH)_2$	20	1489
Chalcedony	SiO_2	16	7052
Calcite	$CaCO_3$	3	812
Analcite	$Na_{0.96}Al_{0.96}Si_{2.04}O_6{:}H_2O$	3	309
Quartz (sand)	SiO_2	18	7934
Porosity	-	40	-
Secondary Minerals			
Ca-saponite	$Ca_{0.165}Mg_3Al_{0.33}Si_{3.67}O_{10}(OH)_2$	-	-
Celadonite	$KMgAlSi_4O_{10}(OH)_2$	-	-
Gyrolite	$Ca_2Si_3O_7(OH)_2{:}1.5H_2O$	-	-
Laumontite	$CaAl_2Si_4O_{12}{:}4H_2O$	-	-
Leucite	$KAlSi_2O_6$	-	-
Muscovite	$KAl_3Si_3O_{10}(OH)_2$	-	-
14Å-Tobermorite	$Ca_5Si_6H_{21}O_{27.5}$	-	

Table A2.12 Bentonite and cement porefluid compositions at 25 °C (from [196])

Determinand	Units	Initial Bentonite Porewater	Initial Cement Porewater
pH		9.26	13.2
Na	mol/kg	3.6E-3	1.15E-1
K	mol/kg	5.6E-8	1.0E-1
Mg	mol/kg	4.3E-10	-
Ca	mol/kg	1.8E-5	2.52E-3
Cl	mol/kg	4E-5	-
S	mol/kg	1.2E-4	1.97E-3
C	mol/kg	2.7E-3	-
Si	mol/kg	1.6E-4	1.22E-4
Al	mol/kg	2.5E-6	3.04E-5

The simulations show that within a few millimetres of the boundary between the bentonite and the cementitious fluid, porosity decreases dramatically owing to precipitation of cementitious phases. At greater distances there is a zone with increased porosity, up to a few tens of centimetres from the boundary. However, still further from the interface, there is a porosity decrease due to precipitation of secondary minerals. The low-porosity zone extends for a few tens of centimetres into the bentonite, before porosity returns to its initial value. These changes are illustrated for a simulation of 1000 years duration in Figure A2-10.

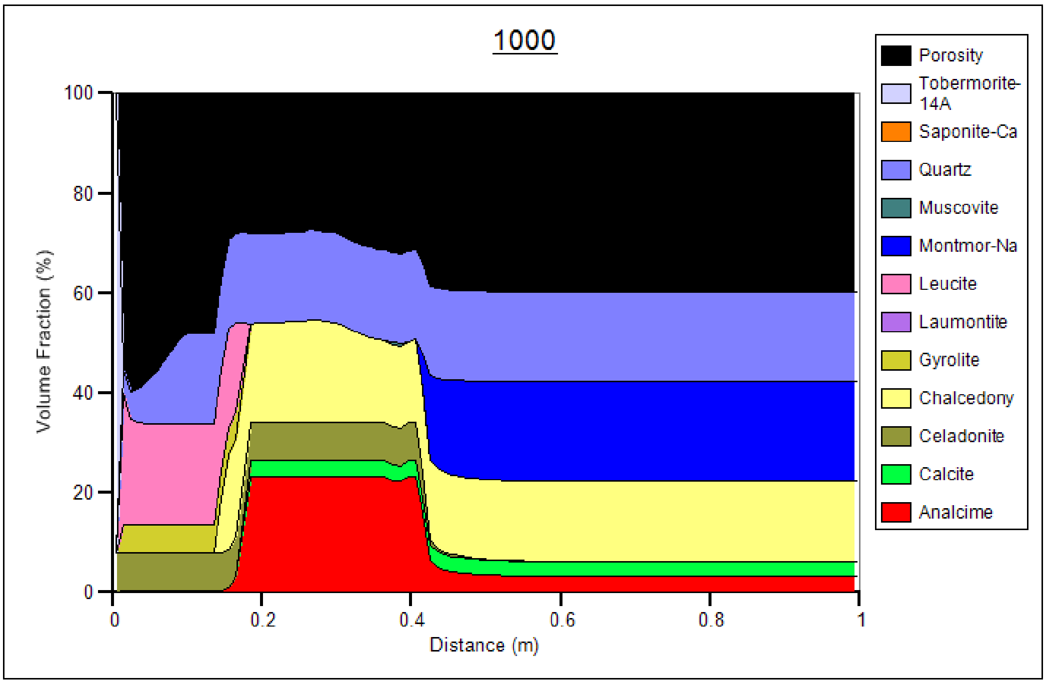


Figure A2-10 Variation in the mineralogical composition of bentonite when exposed to high-pH cement porefluid at one boundary (represented by the left hand axis of the figure), after 1000 years of reaction.

The decrease in porosity at the margin between the cement and the bentonite ultimately leads to mass transport of cementitious porewater into the bentonite slowing to an insignificantly small rate. As a result, the zones of increased and reduced porosity further within the bentonite cease to evolve significantly. The net consequence is that overall the alteration caused by cement-bentonite interactions extends no more than a few tens of centimetres into the bentonite.

An implication is that a cementitious borehole support element will impact upon the performance of an adjacent bentonite-based seal only within a short distance (perhaps up to a few tens of centimetres) from the interface between the two. If the length of the bentonite seal is long compared with this zone (which is almost certain to be the case) then the overall effect on the performance of the seal will be small. Furthermore, on the basis of these calculations, the distance over which the bentonite's performance will be impaired is likely to coincide with the zone of enhanced porosity, which is significantly shorter than the overall distance over which reactions occur. However, it should be noted that these calculations did not consider the effect of the alteration on the mechanical properties of the sealing materials. It is possible that these effects could be detrimental to seal performance, for example if the porosity reduction also makes the seal more brittle and hence more susceptible to fracturing.

Alteration of the kind simulated here would potentially be more significant where a bentonite seal is emplaced adjacent to cement that occurs in the borehole walls. Such cement may have originally formed a bond behind a casing that has since been removed, or alternatively could be grout that has been used to seal fractures. In such cases, a more significant proportion of the bentonite might potentially alter.

A2.5 Uncertainties regarding salinity

All the simulations reported here have considered only fresh and saline groundwater (Table 3-3, Table A2-2). However, in much of the UK deep groundwaters are brines, which are much more saline than the considered saline groundwater, reflecting in large part the widespread distribution of evaporite deposits. A representative brine composition is given in Table 3-3. “Conventional” geochemical models are inappropriate for simulating reactions involving such brines because the models that they use for activity coefficients (commonly either the Davies model or the Debye-Hückel model) become increasingly inaccurate for salinities greater than that of seawater. Instead an alternative approach is needed to calculate activity coefficients in brines. A commonly used approach is the ion interaction approach or “Pitzer approach” (e.g. [226]). However, the thermodynamic data that are required to simulate the behaviour of borehole seals using this approach are unavailable for many of the relevant aqueous species. Furthermore, even where data are available, they are often inapplicable to the full temperature range of relevance.

The potential significance of the limited ability to simulate reactions in the presence of highly saline groundwaters is illustrated by some scoping calculations that are reported in [227]. These authors simulated the water-mineral reactions that would occur in cementitious borehole seals when exposed to CO_2-charged solutions. Although these reactions differ from those that are expected to occur in the sealed site selection boreholes that are the focus of this report, they do illustrate the fact that the choice of thermodynamic database and model used for calculating activity coefficients of aqueous species is potentially important. Figure A2-11shows some key results of this modelling.

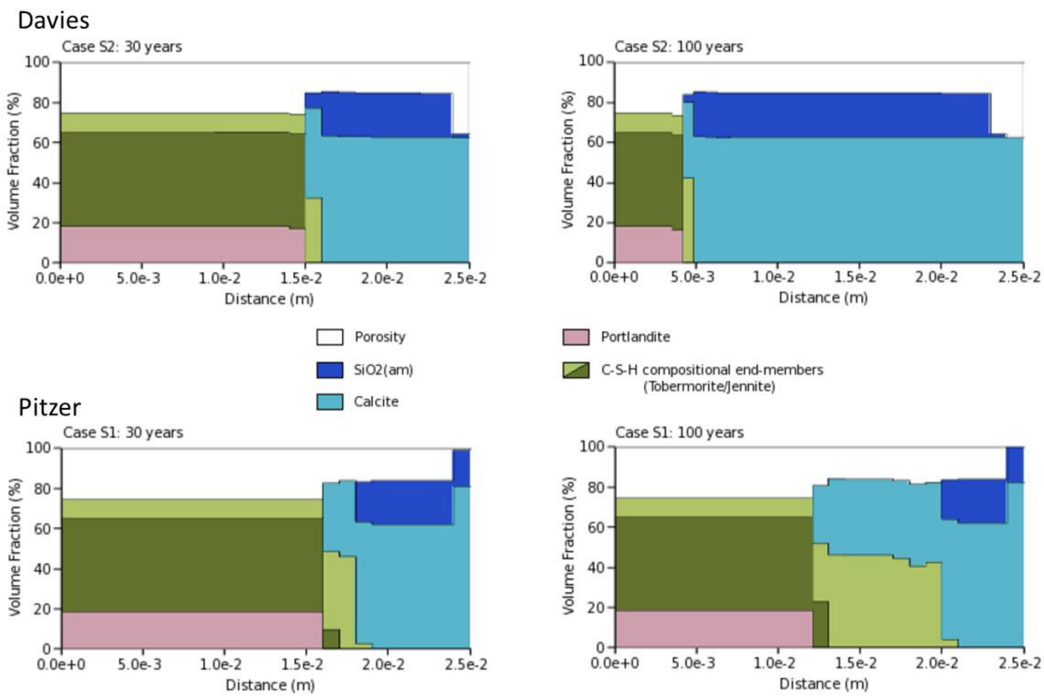


Figure A2.11 Variation in mineral assemblages within cement exposed to CO_2-saturated water when the Davies equation is used to model activity coefficients (above) and when the Pitzer approach is used (below). After [227]

It can be seen that simulations employing both the Davies approach and the Pitzer approach give broadly similar results over short timescales of 30 years. After this time, the results diverge, such that after 100 years of simulation time the results differ markedly. In particular the choice of the Davies model leads to a thicker alteration zone in this model. One implication of these results is that even if models are successful at reproducing short-term observations, for example those obtained from laboratory experiments or field investigations of operating wells, they may not necessarily be reliable in the long term.

A2.7 References

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