Technical Report

TR-10-48

Geosphere process report for the safety assessment SR-Site

Svensk Kärnbränslehantering AB

November 2010

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co

Box 250, SE-101 24 Stockholm
Phone +46 8 459 84 00

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Preface

This document compiles information on processes in the geosphere relevant for long-term safety of a KBS-3 repository. It supports the safety assessment SR-Site, which will support the licence application for a final repository in Sweden.

The work of compiling this report has been led by Kristina Skagius, Kemakta Konsult AB. She has also been the main editor of the report.

The following persons have had the main responsibilities for specific subject areas: Harald Hökmark, Clay Technology AB (thermal and mechanical processes), Jan-Olof Selroos, SKB (hydrogeological and transport processes), and Ignasi Puigdomenech and Birgitta Kalinowski, SKB (geochemical processes).

In addition, a number of experts have contributed to specific parts of the report as listed in Section 1.3.

The report has been reviewed by Jordi Bruno, Amphos, Spain; John Cosgrove, Imperial College, UK; Thomas Doe, Golder Associates Inc, USA; Alan Hooper, Alan Hooper Consulting Limited, UK; John Hudson, Rock Engineering Consultants, UK; Ivars Neretnieks, Royal Institute of Technology, Sweden; Mike Thorne, Mike Thorne and Associates Ltd, UK; and Per-Eric Ahlström, SKB.

Stockholm, November 2010

Allan Hedin

Project leader SR-Site

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1 Introduction

1.1 Role of this process report in the SR-Site assessment

1.1.1 Overall methodology

This report documents geosphere processes identified as relevant to the long-term safety of a KBS-3 repository, and forms an important part of the reporting of the safety assessment SR-Site. The detailed assessment methodology, including the role of the process reports in the assessment, is described in the SR-Site Main report /SKB 2011/. The following excerpts describe the methodology, and clarify the role of this process report in the assessment.

The repository system, broadly defined as the deposited spent nuclear fuel, the engineered barriers surrounding it, the host rock and the biosphere in the proximity of the repository, will evolve over time. Future states of the system will depend on:

- the initial state of the system,
- a number of radiation-related, thermal, hydraulic, mechanical, chemical and biological processes acting within the repository system over time, and
- external influences acting on the system.

A methodology in eleven steps has been developed for SR-Site, as summarised in Figure 1-1 and described below.

1. Identification of factors to consider (FEP processing).

   This step consists of identifying all the factors that need to be included in the analysis. Experience from earlier safety assessments and KBS-3 specific and international databases of relevant features, events and processes (FEPs) influencing long-term safety are utilised. An SKB FEP database is developed where the great majority of FEPs are classified as being either initial state FEPs, internal processes or external FEPs. Remaining FEPs are either related to assessment methodology in general or deemed irrelevant for the KBS-3 concept. Based on the results of the FEP processing, an SR-Site FEP catalogue, containing FEPs to be handled in SR-Site, has been established. This step is documented in the SR-Site FEP report /SKB 2010a/.

2. Description of the initial state.

   The initial state of the system is described based on the design specifications of the KBS-3 repository, a descriptive model of the repository site and a site-specific layout of the repository. The initial state of the fuel and the engineered components is that immediately after deposition, as described in the respective SR-Site Production reports /SKB 2010g, h, i, j, k, l/. The initial state of the geosphere and the biosphere is that of the natural system prior to excavation, as described in the site descriptive model /SKB 2008a/. The repository layout adapted to the Forsmark site is provided in an underground design report /SKB 2009b/.

3. Description of external conditions.

   Factors related to external conditions are handled in the categories “climate-related issues”, “large-scale geological processes and effects” and “future human actions”. The handling of climate-related issues is described in the SR-Site Climate report /SKB 2010c/, whereas the few external, large-scale geosphere processes are addressed here in the Geosphere process report (Section 4.1). The treatment of future human actions in SR-Site is described in the SR-Site FHA report /SKB 2010f/.

4. Compilation of process reports.

   The identification of relevant processes is based on earlier assessments and FEP screening. All identified processes within the system boundary relevant to the long-term evolution of the system are described in dedicated Process reports, i.e. this report and process reports for the fuel and canister /SKB 2010d/ and for the buffer, backfill and closure /SKB 2010e/. Also short-term geosphere processes/alterations, due to repository excavation, are included. For each process, its general characteristics, the time frame in which it is important, the other processes to which it is coupled and how the process is handled in the safety assessment are documented.

Figure 1-1. *An outline of the eleven main steps of the SR-Site safety assessment. The boxes above the dashed line are inputs to the assessment.*

5. Definition of safety functions, function indicators and function indicator criteria.

   This step consists of an account of the safety functions of the system and of how they can be evaluated by means of a set of function indicators that are, in principle, measurable or calculable properties of the system. Criteria for the safety function indicators are provided. The Process reports are important references for this step. A FEP chart is developed, showing how FEPs are related to the function indicators.

6. Compilation of input data.

   Data to be used in the quantification of repository evolution and in dose calculations are selected. The process of selection and the data adopted are reported in a dedicated Data report /SKB 2010b/. Also, a template for discussion of input data uncertainties has been developed and applied.

7. Definition and analysis of reference evolution.

   A reference evolution, providing a description of a plausible evolution of the repository system, is defined and analysed. The isolating potential of the system over time is analysed, yielding a description of the general system evolution and an evaluation of the safety function indicators. Each process is handled in accordance with the plans outlined in the process reports. Radiological consequences of potential canister failures are not analysed in this step.

8. Selection of scenarios.

   A set of scenarios for the assessment is selected. A comprehensive main scenario is defined in accordance with the Swedish Radiation Safety Authority's, SSM's, regulations SSMFS 2008:21. The main scenario is closely related to the reference evolution analysed in step 7. The selection of additional scenarios is focused on the safety functions of the repository, and the safety function indicators defined in step 5 form an important basis for the selection. For each safety function, an assessment is made as to whether any reasonable situation where it is not maintained can be identified. If this is the case, the corresponding scenario is included in the risk evaluation for the repository, with the overall risk determined by a summation over such scenarios. The set of selected scenarios also includes scenarios explicitly mentioned in applicable regulations, e.g. human intrusion scenarios, and scenarios and variants to explore design issues and the roles of various components in the repository.

9. Analysis of scenarios.

   The main scenario is analysed essentially by referring to the reference evolution in step 7, complemented by consequence calculations for potential canister failures in the reference evolution yielding a calculated risk contribution from the main scenario. The additional scenarios are analysed by focussing on the factors potentially leading to situations in which the safety function in question is not maintained. In most cases, these analyses are carried out by comparison with the evolution for the main scenario, meaning that they only encompass aspects of repository evolution for which the scenario in question differs from the main one. If the scenario leads to canister failures, consequence calculations are carried out. If the likelihood of the scenario is non-negligible, a risk contribution is also calculated.

10. Additional analyses.

    In this step, a number of additional analyses, required to complete the safety assessment, are carried out. These comprise e.g. sensitivity analyses of the outcome of the scenario analyses, analyses required to demonstrate optimisation and use of best available technique, analyses of design options alternative to the reference design, analyses supporting risk discussion for the initial 1,000 years and an account of supporting arguments based on natural analogues.

11. Conclusions.

    This step includes integration of the results from the various scenario analyses, development of conclusions regarding safety in relation to acceptance criteria and feedback concerning design, continued site investigations and the R&D programme.

This Geosphere process report is one of the process reports required to complete step 4. The purpose of the process reports is to document the scientific knowledge of the processes to a level required for their adequate treatment in the safety assessment. The documentation is not exhaustive from a scientific point of view, since such a treatment is neither necessary for the purposes of the safety assessment nor possible within the scope of an assessment. However, it must be sufficiently detailed to facilitate, by arguments founded on scientific understanding, the treatment of each process in the safety assessment. The purpose is to determine how to handle each process in the safety assessment at an appropriate degree of detail, and to demonstrate how uncertainties are taken care of, given the suggested handling. The handlings established in this report are used in the analysis of the reference evolution, step 7, and in the analyses of scenarios, step 9.

1.1.2 Identification of processes

The process documentation in this SR-Site process report is an update of the descriptions in the SR-Can version of the Process report /SKB 2006f/. The SR-Can version of the report, in turn, builds on the process documentation in the SR 97 version of the process report /SKB 1999/ and the FEP processing carried out in SR-Can. The complementary FEP processing carried out in SR-Site (step 1 above) did not identify any need to modify the list of relevant processes that were included in the SR-Can version of the geosphere process report /SKB 2006f/, see the SR-Site FEP report /SKB 2010a/ for details. However, one of the processes included in the SR-Can version of the geosphere process report, surface weathering and erosion, has been removed from this SR-Site geosphere process report and instead has been included in the SR-Site Climate report /SKB 2010c/. Furthermore, the names of some processes have been slightly modified as compared to the SR-Can version of the geosphere process report. A complete list of processes described in the SR-Site process reports can be found in the abovementioned FEP report.

1.1.3 Relation to specific sites

SKB has undertaken site characterisation at two different locations, Forsmark and Laxemar-Simpevarp, as candidate sites for a final repository for spent nuclear fuel. The SR-Site assessment builds on site-specific data for, and site-descriptive models of, the selected Forsmark site /SKB 2008a/, but site-specific data for, and site-descriptive models of, the Laxemar site /SKB 2009a/ are also used in evaluations to support the site selection /SKB 2010m/. Therefore, the process descriptions are of a sufficiently general nature to be applicable to both these sites. The result of the quantitative evaluations of the processes in the different scenarios analysed in SR-Site will, in many cases, be dependent on site-specific data. These data are not given here, but in dedicated modelling studies. In addition, the most important data for the safety assessment are thoroughly evaluated in the SR-Site Data report /SKB 2010b/, step 6 above.

1.1.4 Intended audience of this report

This report is written by, and for, experts in the concerned scientific fields. It should though be possible for a generalist in the area of long-term safety assessments of geologic nuclear waste repositories to comprehend the contents of the report. The report is an important part of the documentation of the SR-Site project and an essential reference within the project, providing a scientifically motivated plan for the handling of geosphere processes. It is furthermore foreseen that the report will be essential for reviewers scrutinising the handling of geosphere issues in the SR-Site assessment.

1.2 Structure for process descriptions

All processes identified are documented using a template, where, in essence, all of the headings are the same as those used in the SR-Can version of the report. These are described below.

Overview/general description

Under this heading, a general description of current knowledge regarding the process is given. For most processes, the basis for this is the content of the SR-Can version of the geosphere process report /SKB 2006f/, reviewed and updated as necessary.

Dependencies between process and geosphere variables

For each system component, in this case the geosphere system, a set of physical variables that defines the state of the system is specified (see Section 1.4). For each process, a table is presented under this heading with documentation of how the process is influenced by the specified set of physical variables and how the process influences the variables. In addition, the handling of each influence in SR-Site is indicated in the table.

Boundary conditions

The boundary conditions for each process are discussed. These refer to the boundaries of the geosphere system (see Section 1.4). The processes for which boundary conditions need to be described are, in general, related to transport of material or energy across the boundaries. For example, the discussion of boundary conditions for chemical processes occurring in the geosphere is, in general, related to the boundary conditions of the relevant transport processes occurring in the geosphere, i.e. advection and diffusion.

Model studies/experimental studies

Model and experimental studies of the process are summarised. This documentation constitutes the major source of information for many of the processes.

Natural analogues/observations in nature

If relevant, natural analogues and/or observations in nature that contribute to the present understanding of the process are documented under this heading.

Time perspective

The timescale or timescales over which the process occurs are documented, if such timescales can be defined.

Handling in the safety assessment SR-Site

Under this heading, the handling of the process in the safety assessment SR-Site is described. Typically, the process is either

- neglected on the basis of the information under the previous headings, or
- included by means of modelling.

The following aspects of the handling of the process are covered under this heading, although no prescribed format for the documentation is given.

- Time periods over which the process is relevant for system evolution.
- Handling of boundary conditions, especially any spatial and temporally varying chemical and hydraulic conditions.
- Handling of the interactions between the process and the specified geosphere variables and couplings to other processes within the geosphere system.

The main scenario in SR-Site covers 120,000 years, which is similar to the duration of a Late Pleistocene glacial cycle. Hence, it covers the excavation/operation period, an initial period with temperate climate conditions, and the evolution of periods with periglacial-, temperate- and glacial climate conditions, following the initial temperate period. A future reference glacial cycle based on conditions reconstructed for the last glacial cycle is analysed, together with alternative possible climate developments with a potentially larger impact on repository safety. The climate evolution in e.g. the reference glacial cycle is, after the initial temperate period, described as a time series of climate domains. The climate domains identified as important are the temperate-, periglacial and glacial climate domains, which are defined and described in detail in the SR-Site Climate report /SKB 2010c/. In order to reflect different conditions of relevance for repository performance during the assessment period, the following time periods are addressed in the descriptions of the handling of the processes:

- excavation/operation period,
- initial temperate period,
- periods of periglacial climate domain,
- periods of glacial climate domain.

In addition to this, the handling of the processes in case of earthquakes is specifically addressed. Earthquakes are considered as external events that can affect mechanical processes in the geosphere with subsequent impact on the engineered barrier system, and need to be discussed separately. Earthquakes as events are further discussed in the introduction to the descriptions of mechanical processes (see Section 4.1.3).

Based on the information compiled under this heading in the process descriptions, a mapping of all processes to method of treatment and, in relevant cases, applicable models has been made, see further Section 1.6.

Handling of uncertainties in SR-Site

Given the adopted handling of each process in the safety assessment SR-Site, the handling of different types of uncertainties associated with the process is summarised.

Uncertainties in mechanistic understanding: The uncertainty in the general understanding of the process is discussed based on the available scientific literature and with the aim of addressing whether the basic scientific mechanisms governing the process are understood to the level necessary for the suggested handling.

Model simplification uncertainties: In most cases, the quantitative representation of a process will contain simplifications. These may be a significant source of uncertainty in the description of system evolution. These uncertainties are discussed and approaches to addressing them are identified including alternative models or alternative approaches to simplification of a particular conceptual model.

Input data and data uncertainties: The set of input data necessary to quantify the process for the suggested handling is documented. The further treatment of important input data and input data uncertainties is described in a separate report, the SR-Site Data report /SKB 2010b/, to which reference is made if relevant.

Adequacy of references supporting the handling in SR-Site

Under this heading, statements are provided concerning the adequacy of the references in a quality assurance perspective. These statements are restricted to the references supporting the selected handling and are evaluated in the factual review of the process report, together with the arguments and justifications for the selected handling provided in the preceding subsections.

References

A list of references used in the process documentation is given at the end of the report.

1.3 Participating experts

The experts involved in assembling the basic information on the processes are documented in Table 1-1. The sub-sections "Handling in the safety assessment SR-Site" and "Uncertainties" have been produced by Jan-Olof Selroos, SKB, (flow and transport processes, including diffusion and sorption), Ignasi Puigdomenech and Birgitta Kalinowski, SKB, (geochemical processes), Raymond Munier, SKB (thermal and mechanical processes) and Allan Hedin, SKB, in collaboration with the expert(s) that assembled the information on the process in question. All these experts are included in the SR-Site list of experts as required by the SR-Site QA plan, see further the SR-Site Main report /SKB 2011/.

Table 1-1. Experts responsible for the process documentation.

Process		Expert author, affiliation
2.1	Heat transport	Harald Hökmark, Clay Technology, Sweden
2.2	Freezing	Jens-Ove Näslund, SKB, Sweden Juha Hartikainen, Aalto University School of Science and Technology, Finland
3.1	Groundwater flow	Peter Jackson, Serco Assurance, UK Lee Hartley, Serco Assurance, UK Sven Follin, SF Geologic, Sweden
3.2	Gas flow/dissolution	Peter Jackson, Serco Assurance, UK Lee Hartley, Serco Assurance UK Andrew Hoch, Serco Assurance, UK William Rodwell, Serco Assurance, UK
4.2	Displacements in intact rock	Harald Hökmark, Clay Technology, Sweden
4.3	Reactivation – displacement along existing discontinuities	Harald Hökmark, Clay Technology, Sweden
4.4	Fracturing	Harald Hökmark, Clay Technology, Sweden
4.5	Creep	Harald Hökmark, Clay Technology, Sweden
4.6	Erosion/sedimentation in fractures	Gunnar Gustafson, Chalmers University of Technology, Sweden.
5.2	Advective transport/mixing of dissolved species	Marcus Laaksoharju, Geopoint AB, Sweden
5.3	Diffusive transport of dissolved species in fractures and rock matrix	Martin Löfgren, Niressa AB, Sweden
5.4	Speciation and sorption	James Crawford, Kemakta AB, Sweden
5.5	Reactions groundwater/rock matrix	Björn Sandström, WSP, Sweden
5.6	Dissolution/precipitation of fracture-filling minerals	Björn Sandström, WSP, Sweden
5.7	Microbial processes	Karsten Pedersen, Microbial analytics AB, Sweden
5.8	Degradation of grout	Jorge Molinero, Amphos, Spain
5.9	Colloidal processes	Susanna Wold, Royal Institute of Technology, Sweden
5.10	Formation/dissolution/reaction of gaseous species	Karsten Pedersen, Microbial analytics AB, Sweden
5.11	Methane hydrate formation	John Smellie, Conterra AB, Sweden
5.12	Salt exclusion	John Smellie, Conterra AB, Sweden
5.13	Radiation effects (rock and grout)	John Smellie, Conterra AB, Sweden
5.14	Earth currents	Rolf Sjöblom, Tekedo AB, Sweden
6.1	Transport of radionuclides in the water phase	Jan-Olof Selroos, SKB, Sweden
6.2	Transport of radionuclides in the gas phase	Peter Jackson, Serco Assurance, UK Andrew Hoch, Serco Assurance, UK William Rodwell, Serco Assurance, UK

1.4 Definition of the geosphere system and variables

As mentioned in Section 1.1.3, the SR-Site assessment builds on site-specific data and site-descriptive models of the Forsmark site, although the process descriptions in this report are sufficiently general to cover both sites that have been investigated by SKB, i.e. both Forsmark and Laxemar.

For the purpose of the process descriptions, the geosphere system is defined as the bedrock surrounding and including a potential repository at the sites. The areal extent of the geosphere roughly corresponds to the size of the area investigated at the sites and the vertical extent is down to a depth of about 1,000 m. The inner boundary of the geosphere system is defined as the bedrock interfaces with the buffer in the deposition holes and with the backfill in the deposition tunnels. The outer boundary is the geosphere-biosphere interface, defined as the top of the weathered host rock, which would be either at outcrop or at the interface with Quaternary deposits.

For the purpose of describing the initial state of the geosphere system and how it evolves, as well as for illustrating how different geosphere processes interact, a set of geosphere variables has been defined. These variables are the same as those adopted in the process descriptions of the SR-Can assessment /SKB 2006f/. The variables and their definitions are provided in Table 1-2.

The initial state of the geosphere system is defined as that of the natural system prior to excavation and construction of the repository. Thus, the initial state is provided by the results of the site investigations as documented in the site description of the Forsmark area /SKB 2008a/ and the Laxemar subarea /SKB 2009a/.

Table 1-2. Geosphere variables and their definitions.

Variable	Definition
Temperature in bedrock	Temperature in the bedrock as a function of time and space.
Groundwater flow	Groundwater flow as a function of time and space in the geosphere´s fracture system.
Groundwater pressure	Groundwater pressure as a function of time and space in the geosphere´s fracture system.
Gas phase flow	Gas phase flow as a function of time and space in the geosphere´s fracture system.
Repository geometry	Geometric description of deposition holes, tunnels, ramps, boreholes etc; i.e. of all excavated volumes.
Fracture geometry	All cavities, from fracture zones to micropores in the rock matrix. Also included here is the excavation-disturbed zone (EDZ) and any other geometric changes in the fracture structure induced by construction.
Rock stresses	Rock stresses as a function of time and space.
Matrix minerals	Chemical composition of the rock matrix as a function of time and space, i.e. a description of the various minerals that occur and their extent.
Fracture minerals	Chemical composition of the fracture minerals as a function of time and space, i.e. a description of the various fracture-filling minerals that occur. Also the amount and composition of these fracture-filling minerals.
Groundwater composition	Chemical composition of the groundwater as a function of time and space, i.e. concentrations of relevant components in the groundwater. This variable also includes quantities such as Eh and pH, as well as any radionuclides and dissolved gases.
Gas composition	Chemical composition of gases, including any radionuclides and naturally occurring gases, in geosphere cavities.
Structural and stray materials	Chemical composition and quantities of grouts and other structural and stray materials injected/located in fractures in the rock and left there at repository closure.
Saturation	Degree of water saturation of the geosphere.

1.5 Geosphere performance

In order to evaluate repository performance and long-term safety, a number of safety function indicators and criteria that these should fulfil over time were defined in the SR-Can safety assessment /SKB 2006b/. A safety function is defined qualitatively as a role through which a repository component contributes to safety and a safety function indicator is a measurable or calculable quantity through which a safety function can be quantitatively evaluated /SKB 2006b/. Safety functions and safety function indicators are also applied in SR-Site and are further described in the SR-Site main report /SKB 2011, Chapter 8/.

In order to determine whether a safety function is maintained or not, it is desirable to have quantitative criteria against which the safety function indicators can be evaluated over the time period covered by the safety assessment. Such safety function indicator criteria can be formulated for some geosphere safety functions, whereas others cannot be captured by simple criteria, since they require more complex analyses where the combined effect of a number of factors determines the outcome. The safety functions and safety function indicators and criteria for the geosphere are listed in Table 1-3 together with their motivation.

Table 1-3. Summary of geosphere function indicators and criteria.

Safety function	**Function indicator; *criteria***	**Rationale**	**Reference**
Favourable chemical conditions	Reducing conditions; *Eh limited*	Limit canister corrosion and fuel dissolution.	Fuel and canister process report /SKB 2010d/.
	Salinity; *TDS limited*	Maintaining buffer and backfill properties.	Buffer, backfill and closure process report /SKB 2010e/.
	Ionic strength; $\Sigma q[M^{q+}] > 4\ mM$	Maintaining buffer and backfill properties.	Buffer, backfill and closure process report, /SKB 2010e/.
	Concentration of HS^-, H_2, CH_4, organic carbon, K and Fe; *limited*	Limit canister corrosion. Maintaining buffer and backfill properties.	Fuel and canister process report /SKB 2010d/. Buffer, backfill and closure process report /SKB 2010e/.
	pH; $pH<11$	Maintaining buffer and backfill properties.	Buffer, backfill and closure process report /SKB 2010e/.
	Concentration of Cl and pH; $pH>4$, *or* $[Cl^-] < 3M$	Avoid chloride corrosion.	Fuel and canister process report /SKB 2010d/.
Favourable hydro-logical and transport conditions	Transport resistance in fractures, F; *high*	Contribute to retardation.	Section 6.1 in this report.
	Equivalent flow rate at buffer/rock interface; Q_{eq} *low*	Transport resistance at buffer/rock interface.	Buffer, backfill and closure process report /SKB 2010d/. Section 3.1 in this report.
	Sorption, K_d, matrix diffusion, D_e; *high*	Contribute to retardation.	Sections 5.3, 5.4 and 6.1 in this report.
	Colloid concentration; *low*	Limit radionuclide transport.	Sections 5.9 and 6.1 in this report.
Stable mechanical conditions	Shear movements at deposition holes; < *0.05 m*	Maintain canister integrity.	Fuel and canister process report /SKB 2010d/. Section 4.3 in this report.
	Shear velocity at deposition holes; < *1 m/s*	Maintain canister integrity.	Fuel and canister process report /SKB 2010d/. Section 4.3 in this report.
	Groundwater pressure; limited	Maintain canister integrity.	Fuel and canister process report /SKB 2010d/.
Favourable thermal conditions	Temperature; > −4°C	Avoid buffer freezing.	Buffer, backfill and closure process report /SKB 2010d/. Sections 2.1 and 2.2 in this report.
	Temperature; > 0°C	Maintain canister integrity.	Fuel and canister process report /SKB 2010d/. Sections 2.1 and 2.2 in this report.

1.6 Summary of handling of processes in SR-Site

Table 1-4 summarises the handling of geosphere processes in the safety assessment SR-Site, as suggested in this report. In the table, the process is either “mapped” to a model by which it will be quantified or associated with a brief verbal description of how it will be handled. Acronyms and model names are explained in Appendix A.

Table 1-4. Process table for the geosphere describing how processes will be handled in different time frames/climate domains and in the special case of earthquakes. Green fields denote processes that are neglected or irrelevant. Red fields denote processes that are quantified by modelling in the safety assessment. Orange fields denote processes that are neglected subject to a specified condition.

Process	Excavation/ operation	Temperate	Periglacial	Glacial	Earthquakes
Ge1 Heat transport	Neglected since sensitivity studies show that it takes very specific excavation/ deposition sequences for heat generation to influence.	Modelling of peak canister temperature, assesment of distribution of peak temperature among the canisters and temperature distribution in rock.	Site-specific 2-D estimations of temperature distribution with depth.	Site-specific 1-D estimations of sub-glacial permafrost- and freezing depths.	Not relevant.
Ge2 Freezing	Not relevant.	Not relevant.	Site-specific 2-D estimations of permafrost- and freezing depths.	Site-specific 1-D estimations of sub-glacial permafrost- and freezing depths.	Not relevant.
Ge3 Groundwater flow	Modelling of inflow, water table drawdown and salt water upconing assuming saturated groundwater flow using DarcyTools. MIKE SHE used for simulating water table drawdown effects in detail.	Modelling of backfill resaturation using DarcyTools and saturated groundwater flow on different scales using ConnectFlow.	Modelling of saturated groundwater flow on a super-regional scale using DarcyTools.	Modelling of groundwater flow on a super-regional scale during advance and retreat of ice sheets, with and without permafrost, using DarcyTools.	Impact on groundwater flow not specifically addressed but simplified calculations of radionuclide transport carried out (see Ge24).
Ge4 Gas flow/ dissolution	Neglected based on arguments supporting the assumption of small effects of unsaturated regions on inflows to tunnels.	Included in a simplified manner in the backfill resaturation calculations. Neglected for other calculations based on the assumption that gas generated in the repository can rapidly escape through the geosphere without causing a pressure build-up.	Neglected in SR-Site based on considerations that gas that may be trapped below permafrost will have a similar effect on groundwater flow to a slightly thicker permafrost layer. Also, gas may escape through taliks if present.	Neglected in SR-Site based on the assumption that gas generated in the repository can rapidly escape through the geosphere without causing a pressure build-up (if permafrost is not present).	Not relevant.

Process	**Excavation/ operation**	**Temperate**	**Periglacial**	**Glacial**	**Earthquakes**
Ge5 Displacements in intact rock	3DEC modelling of near-field effects of excavation of tunnels and deposition holes.	3DEC modelling of thermal stresses and deformations in the near field and in the far field.	3DEC modelling of horizontal stress reduction caused by cooling.	3DEC stress modelling of near field. ABAQUS modelling of far field.	Included in the modelling of shear movements.
Ge6 Reactivation – displacement along existing discontinuities	3DEC modelling of construction-induced reactivation. Construction-induced seismicity neglected since extraction rate is too small to generate anything but local and limited construction-induced potential instability.	3DEC modelling of reactivation due to thermal load (near field). Assessment of reactivation based on 3DEC stress evolution (far field). Estimation of earthquake probability (consequence analysis, see Earthquake).	3DEC modelling of fracture reactivation caused by thermal stress reduction, forebulge stress conditions and pore overpressure under impermeable permafrost layer (near field). Assessment of reactivation based on ABAQUS stress evolution, 3DEC thermal stress reduction and pore overpressure estimates (far field). Estimation of earthquake probability (consequence analysis, see Earthquake).	3DEC modelling of ice-load induced reactivation. Assessment of reactivation based on ABAQUS stress model and pore overpressure estimates. Estimation of earthquake probability (consequence analysis, see Earthquake).	Apply design rules (respect distances and canister spacing). Assessment of residual probability for canister failure due to shear displacement.
Ge7 Fracturing	Assessment of EDZ. 3DEC modelling of potential for spalling. Observations of size and shape of fractured (spalled) zone around deposition holes.	3DEC modelling of potential for spalling. Observations (APSE) of size and shape of fractured (spalled) zone around deposition holes.	Thermal effects modelled and neglected provided that only marginal changes in mechanical state occur. Assessment of hydraulic fracturing under impermeable permafrost layer.	3DEC modelling of potential for fracturing induced by ice load (near field). Assessment of risk of hydraulic fracturing.	Neglected based on lack of observations at relevant distances from earthquake faults of earthquake-induced damage around open tunnels at shallow depth.
Ge8 Creep	Not relevant. Covered by construction-induced reactivation.	Neglected because of insignificant convergence of deposition holes at expected rock stresses.	Neglected because of insignificant convergence of deposition holes at expected rock stresses.	Neglected because of insignificant convergence of deposition holes at expected rock stresses.	Not relevant
Ge9 Surface erosion and weathering	The description of the handling of this process has been moved to the Climate report /SKB 2010c/. (Index numbers of subsequent processes not changed to ensure compatibility with the FEP report /SKB 2010a/.)				
Ge10 Erosion/ sedimentation in fractures	Neglected because of too low flow rates in non-grouted fractures.	Neglected because expected hydraulic gradients and shear stresses are too low to cause significant erosion.	Neglected because expected hydraulic gradients and shear stresses are too low to cause significant erosion.	Neglected because expected hydraulic gradients and shear stresses are too low to cause significant erosion.	Not relevant

Process	**Excavation/operation**	**Temperate**	**Periglacial**	**Glacial**	**Earthquakes**
Ge11 Advective transport/mixing of dissolved species	Advection and dispersion of salt included in saturated groundwater flow modelling using DarcyTools. Composition of mixtures assessed based on the groundwater flow modelling and site understanding.	Advection and dispersion of salt and reference waters included in saturated groundwater flow modelling using ConnectFlow. Composition of mixtures assessed based on the groundwater flow modelling and site understanding.	Advection and dispersion of salt included in saturated groundwater flow modelling using DarcyTools. Composition of mixtures assessed based on the groundwater flow modelling and site understanding.	Advection and dispersion of salt included in saturated groundwater flow modelling using DarcyTools. Composition of mixtures assessed based on the groundwater flow modelling and site understanding. Modelling of oxygen penetration based on the groundwater flow modelling, matrix diffusion and reactions with matrix minerals.	Not relevant
Ge12 Diffusive transport of dissolved species in fractures and rock matrix	Diffusion of salt between mobile and immobile groundwater included in saturated groundwater flow modelling using DarcyTools.	Diffusion of salt between mobile and immobile groundwater included in saturated groundwater flow modelling using ConnectFlow.	Diffusion of salt between mobile and immobile groundwater included in saturated groundwater flow modelling using DarcyTools.	Diffusion of salt between mobile and immobile groundwater included in saturated groundwater flow modelling using DarcyTools. Modelling of oxygen penetration based on the groundwater flow modelling, matrix diffusion and reactions with matrix minerals.	Not relevant.
Ge13 Speciation and sorption	Not relevant.	Simplified K_d-approach for modelling sorption of radionuclides. Speciation considered in the selection of K_d values	Simplified K_d-approach for modelling sorption of radionuclides. Speciation considered in the selection of K_d values	Simplified K_d-approach for modelling sorption of radionuclides. Speciation considered in the selection of K_d values	Not relevant.
Ge14 Reactions groundwater/rock matrix	Neglected since reactions are considered to be insignificant compared with the effects of reactions with fracture-filling minerals.	Neglected since reactions are considered to be insignificant compared with the effects of reactions with fracture-filling minerals.	Neglected since reactions are considered to be insignificant compared with the effects of reactions with fracture-filling minerals.	Modelling of oxygen penetration based on the groundwater flow modelling, matrix diffusion and reactions with matrix minerals.	Not relevant

Process	Excavation/ operation	Temperate	Periglacial	Glacial	Earthquakes
Ge15 Dissolution/ precipitation of fracture-filling minerals	Composition of groundwater in fractures modelled based on results of the groundwater flow modelling, assumed local mineral equilibria and site understanding.	Composition of groundwater in fractures modelled based on results of the groundwater flow modelling, assumed local mineral equilibria and site understanding.	Composition of groundwater in fractures modelled based on results of the groundwater flow modelling, assumed local mineral equilibria and site understanding.	Composition of groundwater in fractures modelled based on results of the groundwater flow modelling, assumed local mineral equilibria and site understanding. Reactions with oxygen are considered in the analyses of oxygen penetration	Not relevant
Ge16 Microbial processes	Modelling of diffusive transport of methane and hydrogen, mass balance calculations of organic matter and assessment of potential for microbial processes.	Modelling of diffusive transport of methane and hydrogen, mass balance calculations of organic matter and assessment of potential for microbial processes.	Modelling of diffusive transport of methane and hydrogen, mass balance calculations of organic matter and assessment of potential for microbial processes.	Modelling of diffusive transport of methane and hydrogen, mass balance calculations of organic matter and assessment of potential for microbial processes.	Not relevant.
Ge17 Degradation of grout	Neglected since expected effects will occur during Temperate period.	Generic modelling of effects on chemistry of fractures and changes of hydraulic conductivity in grouting boreholes.	Not specifically handled. Extrapolation of results from Temperate period	Not specifically handled. Extrapolation of results from Temperate period	Not relevant.
Ge18 Colloidal processes	Neglected because of insignificant impact on geochemical conditions.	Neglected because of insignificant impact on geochemical conditions.	Neglected because of insignificant impact on geochemical conditions.	Neglected because of insignificant impact on geochemical conditions.	Impact of earthquakes on colloidal processes not addressed, but simplified calculations of radionuclide transport carried out (see Ge24).
	Impact on radionuclide transport not relevant because of intact barriers.	Bounding calculations of colloid-facilitated radionuclide transport performed.	Bounding calculations of colloid facilitated radionuclide transport performed.	Bounding calculations of colloid facilitated radionuclide transport performed.	
Ge19 Formation/ dissolution/ reaction of gaseous species	Composition of mixtures modelled based on the groundwater flow modelling, assumed local mineral equilibria and site understanding. This affects the concentrations of dissolved CO_2.	Modelling of diffusive transport of methane and hydrogen.	Modelling of diffusive transport of methane and hydrogen.	Included in modelling of oxygen consumption. Modelling of diffusive transport of methane and hydrogen.	Not relevant.
Ge20 Methane hydrate formation	Not relevant.	Not relevant.	Neglected based on site understanding coupled with assessment of the potential for hydrate formation.	Neglected based on site understanding coupled with assessment of the potential for hydrate formation.	Not relevant.

Process	Excavation/ operation	Temperate	Periglacial	Glacial	Earthquakes
Ge21 Salt exclusion	Not relevant.	Not relevant.	Modelling of transport of outfrozen salt.	Not relevant	Not relevant.
Ge22 Radiation effects (rock and grout)	Neglected because of too low radiation fluxes.	Neglected because of too low radiation fluxes.	Neglected because of too low radiation fluxes.	Neglected because of too low radiation fluxes.	Not relevant.
Ge23 Earth currents	Neglected since expected electrical potential fields are too small to affect groundwater flow or solute transport.	Neglected since expected electrical potential fields are too small to affect groundwater flow or solute transport.	Neglected since expected electrical potential fields are too small to affect groundwater flow or solute transport.	Neglected since expected electrical potential fields are too small to affect groundwater flow or solute transport.	Not relevant.
Ge24 Transport of radionuclides in the water phase	Not relevant since engineered barriers are intact.	Advection, dispersion, matrix diffusion, sorption, and radioactive decay included in integrated modelling using FARF31 and MARFA.	Advection, dispersion, matrix diffusion, sorption, and radioactive decay included in integrated modelling using FARF31 and MARFA.	Advection, dispersion, matrix diffusion, sorption, and radioactive decay included in integrated modelling using FARF31 and MARFA.	No credit taken for radionuclide retention in the geosphere i.e.geosphere far field is short-circuited.
Ge25 Transport of radionuclides in the gas phase	Not relevant since engineered barriers are intact.	Assessed by neglecting the geosphere as a barrier.	Assessed by neglecting the geosphere as a barrier.	Assessed by neglecting the geosphere as a barrier.	Not relevant

1.7 Handling of FEPs mapped to the geosphere process system

As a point of departure for the safety assessment SR-Can, a processing of features, events and processes, FEPs, of relevance for the long-term safety of a KBS-3 repository was carried out /SKB 2006c/. For SR-Site, a complementary processing was undertaken, focussing on new NEA project FEPs included in a later version of the international NEA FEP database. This work is further described in the SR-Site FEP report /SKB 2010a/.

As mentioned above, the complementary FEP processing has not led to any revision of the list of geosphere processes compared with those treated in the previous SR-Can assessment.

The complementary FEP processing has also provided lists of project FEPs in the international NEA FEP database version 2.1 that are related to the different geosphere processes. These lists are essentially the same as those developed for SR-Can based on version 1.2 of the NEA FEP database, except that the updated lists also contain all new project FEPs in the later version (2.1) of the NEA FEP database. As in SR-Can, these FEP lists have been used by the experts developing the process descriptions, in order to ensure that all relevant aspects of a process are addressed in the process descriptions and appropriately handled in the SR-Site assessment. The handling of each FEP has been documented by the experts involved in developing the process descriptions in tables created for this purpose. These tables are provided in the SR-Site FEP report /SKB 2010a/ and the handling is also documented in the SKB FEP database.

In general, the results of these checks showed that all relevant NEA project FEPs were already covered by the process descriptions and included in existing plans for how to handle the associated processes in the SR-Site assessment.

2 Thermal processes

2.1 Heat transport

2.1.1 Overview/general description

Heat transport, i.e. transport of thermal energy between two points of differing temperature, can take place by conduction, flow (convection) or radiation. Heat can also be transmitted between different phases in conjunction with condensation and evaporation. Under steady-state (time-independent) conditions, the heat transport in solid phases is determined solely by the thermal conductivity λ of the medium. Under transient (time-dependent) conditions, the heat storage capacity of the medium is also a factor, given by the specific heat capacity, c, and the density, ρ. In general, temperature propagation in solids can be designated as a diffusion process with the diffusion constant (thermal diffusivity) $\alpha = \lambda/(c{\cdot}\rho)$.

For determining the temperature evolution in the bedrock, heat transport in the geosphere can be equated with heat transport in rock. The volumes of other material present in soil strata at the ground surface or in altered fracture zones, where the principle of heat transport differs somewhat from that in the rock, are far too limited to be of importance for the thermal evolution in the host rock. Crystalline rock generally has a low permeability, which means that heat transport takes place principally by conduction. Convection occurs, but it can easily be shown that the low flow rates in the rock and the low mean porosity together make the contribution of convection negligible, see e.g. /Thunvik and Braester 1980/. Furthermore, disregarding the contribution from convection means that the thermal conductivity is underestimated and thus the temperatures are overestimated. The above means that the heat transport mechanism that is relevant for the safety assessment is heat conduction in intact rock and that determination of values of the conductivity λ and the diffusivity α for different rock types and for differently sized volumes of rock of different composition is a key issue for an appropriate handling of the process. Heat transport is also discussed in relation to freezing (Section 2.2) and the development of permafrost as described in the SR-Site Climate report /SKB 2010c/.

Natural heat transport takes place in the Earth's crust from deeper, hotter parts to the Earth's surface, where cooling takes place by heat transfer to the atmosphere. In crystalline bedrock, heat is also generated by radioactive decay in the rock material. Below depths to which thermal effects of glacial cycles can reach, the geothermal heat flow is approximately at steady-state and is, therefore, determined by the rock's thermal conductivity and by the geothermal gradient. The latter provides a measure of the variation of the temperature with depth. At a depth of 500 m, the temperature is between 5.5°C and 14.5°C in Swedish bedrock /Ahlbom et al. 1995/.

The natural temperature conditions at great depths are to be regarded as very stable in a long time perspective. Near the ground surface and down to a depth of several hundred metres there is a climatic impact on the temperature gradients. The variations are the result of colder conditions during past glacial episodes (see the SR-Site Climate report /SKB 2010c/).

Heat generated by the spent nuclear fuel will give rise to a temperature perturbation that propagates in all directions from the repository. Heat conduction in rock is roughly linear, i.e. with heat transport properties being approximately independent of the temperature, so the heat flow from the repository is independent of the geothermal heat flow and will be superimposed on it. The process is transient and determined by the total thermal power output of the repository, by the power distribution, which varies in both space and time, and by the thermal diffusivity of the rock. The thermal output declines with time in accordance with known power-time relationships /Thunvik and Braester 1991, Hökmark et al. 2009/. After 100 years, the decay power will have been reduced by about 70%. At a repository depth of about 500 m, the thermal perturbation will reach the ground surface approximately three hundred years after deposition.

2.1.2 Dependencies between process and geosphere variables

Table 2-1 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 2.1.7.

Table 2-1. Direct dependencies between the process "Heat transport" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Temperature in bedrock	Yes. Temperature gradients are the driving force for heat transport. Thermal conductivity and heat capacity are temperature dependent.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	Yes.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).
		Temperate	Site-specific temperature and thermal properties. Dependence of thermal properties on T accounted for in dimensioning calculations. Otherwise thermal properties for constant T.		Temperate	Output from calculations.
		Periglacial Glacial	See Temperate above and Climate report /SKB 2010c/.		Periglacial Glacial	Output from calculations, see also Section 2.2 Freezing and Climate report /SKB 2010c/.
Groundwater flow	Yes.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No. But indirectly through temperature.	–	See Section 3.1 Groundwater flow.
		Temperate Periglacial Glacial	Influence of convection neglected; little significance.			
Groundwater pressure	Yes.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No. But indirectly through temperature.	–	See Section 3.1 Groundwater flow.
		Temperate	Influence neglected; little significance.			
		Periglacial Glacial	See Temperate above and Climate report /SKB 2010c/.			
Gas phase flow	Yes.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No. But indirectly through temperature.	–	See Section 3.2 Gas flow/dissolution.
		Temperate	Influence neglected; little significance.			
		Periglacial Glacial	See Temperate above and Climate report /SKB 2010c/.			
Repository geometry	Yes. Affects heat flux from repository. Canister spacing particularly important in the near field.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No.	–	–
		Temperate	Included in model.			
		Periglacial Glacial	Included in permafrost model (Climate report /SKB 2010c/).			
Fracture geometry	Yes.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No. But indirectly through rock stresses and temperature.		See mechanical processes in Chapter 4.
		Temperate	Influence neglected; little significance.			
		Periglacial Glacial	Influence neglected; little significance.			
Rock stresses	No.	–	–	No. But indirectly through temperature.		See mechanical processes in Chapter 4.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Matrix minerals	Yes. Determines thermal properties.	Excavation/ operation Temperate Periglacial Glacial	Heat transport neglected (see Section 2.1.7). Use of site-specific thermal properties. Use of site-specific thermal properties in permafrost model /SKB 2010c/.	No.	–	–
Fracture minerals	Yes. Marginally and locally.	Excavation/ operation Temperate Periglacial Glacial	Heat transport neglected (see Section 2.1.7). Influence neglected; little significance. Influence neglected; little significance. /SKB 2010c/	No. But indirectly through temperature and groundwater composition.	–	See chemical processes in Chapter 5.
Groundwater composition	No.	–	–	No. But indirectly through temperature.	–	See chemical processes in Chapter 5.
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	Yes. Affects scope and extent of convective heat transport	Excavation/ operation Temperate Periglacial Glacial	Heat transport neglected (see Section 2.1.7). Influence neglected; little significance. See Temperate above and Climate report /SKB 2010c/.	No. But, indirectly through temperature.	–	–

Temperature in bedrock; Heat transport affects the temperature in all parts of the geosphere. Temperature differences between different points in space comprise the driving force for heat transport. The thermal conductivity and heat capacity of rocks are both slightly temperature dependent. For the Forsmark and Laxemar rock types, the conductivity decreases by about 10% per 100°C /Back et al. 2007, Sundberg et al. 2008a/. In the region nearest a canister, the maximum temperature increase can amount to 45–50°C, which means that the thermal conductivity is reduced at most by about 10%. At a distance of a few metres from the deposition holes, the reduction is much less. The rock heat capacity increases by typically 25% per 100°C, but this parameter is relatively unimportant for the maximum temperatures reached in the near field. In addition, ignoring the increase is pessimistic. The approximation that is often made in rock temperature calculations, namely that the heat transport properties are temperature-independent, can, therefore, be justified.

Groundwater flow; Heat transport will give rise to temperature gradients and density changes that affect large-scale circulatory water movements /Claesson 1992, Probert 1998, Löfman 2005/. This effect will have limited influence on the flow pattern (cf. Section 3.1 Groundwater flow). The groundwater flow contributes to the heat transport, but because of the low permeability and the low flow rates, this contribution is sufficiently small to be ignored in comparison with the conductive heat transport /Thunvik and Braester 1980/.

Groundwater pressure; Heat transport will influence groundwater temperature which, in turn, will influence groundwater pressure. In contrast to the conditions in argillaceous rocks, the hydraulic conductivity of crystalline rocks will be sufficient to dissipate thermally induced increases in pore pressure. /Selvadurai and Nguyen 1997/, for instance, showed that the thermally-induced fluid pressure around a repository located 1,000 m below ground surface, with a significantly higher thermal load than the KBS-3 repository at Forsmark and with a hydraulic conductivity of $1 \cdot 10^{-11}$m/s at all depths, was only about 2 MPa. Between the repository and the ground surface at Forsmark, the large-scale hydraulic conductivity is orders of magnitude higher and the distance to the ground surface less than half that of the repository considered in the model analysed by /Selvadurai and Nguyen 1997/. This means that any thermally induced fluid pressures in Forsmark will be much less and can be ignored. The groundwater pressure cannot have any influence on the heat transport.

Gas phase flow; The influence of gas flow on heat transport in the geosphere is negligible.

Repository geometry; The repository geometry is important for the way the heat generated by the decaying fuel is transported. The spacings between individual spent fuel canisters and between deposition tunnels must be set at values that ensure that the heat dissipation is sufficient to keep the canister temperatures below the design limits /Hökmark et al. 2009/. For the design limits, the most important geometrical parameter is the distance between neighbouring canisters. For the general large-scale heat flow pattern, the power density and the number of repository layers are important.

Fracture geometry; Heat transport will not have any important influence on the fracture geometry. However, there may be some fracture propagation close to excavated openings (see Section 4.4). The presence of fractures reduces the thermal conductivity, particularly if the fractures are filled with air ($\lambda \approx 0.025$ W/(m·K)). However, air-filled fractures represent such a small fraction of the total volume that the effect can be neglected. For water-filled fractures, $\lambda = 0.6$ W/(m·K), which together with the low porosity means that this influence can also be neglected.

Rock stresses; Heat transport is important for the way thermal stresses are induced. When stresses increase, fractures are compressed, which may marginally increase the thermal conductivity. The effect is small and can be neglected.

Matrix minerals; The process will not influence the mineral composition of the rock matrix. The mineral composition of the individual rock types is important in determining the thermal conductivity and the rock heat capacity of the rock. In particular the heat conductivity is decisive for the determination of the canister spacing in the different rock units. This parameter has been extensively measured in the site-investigation programme and models for the effects of spatial variations have been developed /Back et al. 2007, Sundberg et al. 2008a, b/. The models have been applied to establish the layout D2 canister and tunnel spacing at the Forsmark and Laxemar sites /SKB 2009d, e/.

Fracture minerals; Heat transport and the subsequent temperature variation will affect fracture mineralogy. For example, Fe(III) oxyhydroxides will age to either hematite or goethite and clays. Alterations are likely to be found mainly in the near field where temperatures are high. Possible effects on, for instance, fracture transmissivities would be small compared to effects of mechanically induced aperture changes.

Groundwater composition; The temperature may impede or promote reactions in the groundwater.

Gas composition; There will be some increase in water vapour content during the time before the near field is fully saturated. Otherwise, there are no influences on the composition of the gas phase. The gas phase composition does not influence the heat transport.

Structural and stray materials; The volumes that possibly could be occupied by structural and stray materials are too small to influence the heat transport.

Saturation; The thermal expansion of the water in unsaturated regions close to the excavated opening will increase the saturation. The temperature will influence the relative humidity and contribute to control of the vapour-liquid equilibrium.

2.1.3 Boundary conditions

Influence of the boundaries

Prevailing and past climatic conditions, geothermal heat flow, including radiogenic heat production, and the thermal properties of the rock determine the initial temperature and temperature gradients (see also Climate-related issues Section 3.4 Permafrost in the SR-Site Climate report /SKB 2010c/). The ground surface acts as a cooled boundary, contributing towards reducing the temperatures in the repository host rock. However, the effects of heat generated by the spent fuel do not reach the ground surface until long after the temperatures in the near field have begun to decrease. The maximum temperature in the near field is, therefore, not affected by conditions at the ground surface.

The bentonite buffer transfers the heat generated in the canister to the rock. The buffer-rock interface acts, consequently, as a boundary for the geosphere. A few weeks after deposition, the heat front has reached and passed the boundary of the deposition hole. After that, the heat flow through the buffer is quasi-steady-state, i.e. heat is transferred to the rock at the same rate as it is generated in the canister. Therefore, the heat transport properties of the buffer and the canister are without importance for the temperatures in the rock after a few weeks.

The tunnel backfill can be estimated to have a thermal conductivity of about 1.0 W/(m·K) and, therefore, slightly reduces the average thermal conductivity in the near field. The actual value of the thermal conductivity will depend on the backfill composition. However, the volume of the tunnels in relation to that of the near field is so small that the effect can be neglected /Hökmark et al. 2009/. The small importance of the tunnel backfill for heat transport is illustrated by the model calculations done for the Prototype Repository in the Äspö Hard Rock Laboratory (HRL) /Kristensson and Hökmark 2007/.

Influence on the surface

Heat transport has a marginal influence on the thermal conditions at the ground surface. The time integral of the thermal power expression describing the decaying heat generation (cf. /Hökmark et al. 2009/) gives the thermal energy that is generated during a given period of time. If it is assumed that 6,000 canisters are deposited with an initial power output of 1,700 W each, a thermal energy of approximately 17 TWh is evolved during the first 1,500 years after deposition. If all of this energy reaches the ground surface and is transferred to the atmosphere during the period 500–1,500 years after deposition, the annual energy contribution is not larger than that from 850 detached homes, each with an annual gross energy consumption of 20,000 kWh.

Importance for thermal evolution in fuel, buffer and canister

For a given canister power and deposition geometry, the heat transport in the rock is decisive for the temperature at the deposition hole boundary and thereby for the temperature in the buffer and in the canister. This is the most important safety-related aspect of the process of heat transport in the geosphere.

The temperature at the boundary of the deposition hole will act as a boundary condition for the heat flow in the buffer and thereby be decisive – together with the heat transport properties of the buffer, the canister power and open, air-filled gaps – for the temperature on the canister surface and in the buffer. With the analytical calculation method described below under “Model studies”, the temperature in the near field, for example at the deposition hole boundary, can be calculated for different assumptions regarding the heat conduction properties of the rock, the deposition geometry and the deposition sequence.

2.1.4 Model studies/experimental studies

Model studies presented here treat the transport from the repository of the heat generated by the spent nuclear fuel. Model studies related to heat transport during other periods: periglacial, glacial, are described in the SR-Site Climate report /SKB 2010c/.

Numerical temperature calculations with a FEM code have been done by /Thunvik and Braester 1991/. Furthermore, several numerical temperature calculations have been done in conjunction with thermo-mechanical analyses, see e.g. /Hakami et al. 1998, Fälth and Hökmark 2007/. The thermal evolution of the Prototype Repository rock mass has been calculated in great detail by /Kristensson and Hökmark 2007/. The calculation results were found to agree very well with measured rock mass temperatures, giving support to the notion that the heat transport process in repository rock is well understood and can be handled adequately. A numerical scheme for calculation of the early thermal evolution in the near field which takes full account of the spatial variability of the heat transport properties is described and exemplified in /Hökmark et al. 2009/.

/Claesson and Probert 1996/ developed a system for analytically calculating the temperature at an arbitrary point in the host rock as a function of time after deposition. The method was applied to a KBS-3 type repository by /Probert and Claesson 1997/ and further developed by /Hökmark et al. 2009/. The repository is assumed to be designed as one or more rectangular areas. Both the temperature at large distances from the repository and the temperature in the area between tunnels and deposition holes can be calculated. Input data to the calculation are the heat transport properties of the rock, the power output of the canisters at the time of deposition, the height of the canister, the power decay, the depth below the ground surface and the deposition geometry, i.e. tunnel spacing and canister spacing. It is assumed in the analytical solution that the rock is homogeneous and continuous and that the rock heat transport properties are independent of the temperature. The analytical solution can be used to analyse effects of distributing the deposition over time. The analytical solution has been verified by comparison with results from numerical calculation of the rock temperature in the near field in a KBS-3 repository /Fälth and Hökmark 2007, Hökmark et al. 2009/. Figure 2-1 shows analytically calculated temperatures at three points in the near field.

2.1.5 Natural analogues/observations in nature

Not applicable.

2.1.6 Time perspective

The maximum rock temperature, 45–50°C above the undisturbed temperature, will be found at the walls of the deposition holes some 30 years after deposition /Hökmark et al. 2009/. Ten thousand years after deposition, the heat generation will have dropped by about 99%. However, because of the relatively low rock heat conductivity, the temperature will still be 5–8°C above the initial undisturbed rock temperature at the depth of the repository. After another 10,000 years, the heat flow in the repository rock will be determined by the natural geothermal conditions. A few thousand years after deposition, the thermal gradients within the repository region will be very small. However, the heat generated by the spent fuel will have an impact on the development of permafrost (by definition the 0°C isotherm) even 100,000 years after closure, see the SR-Site Climate report /SKB 2010c/.

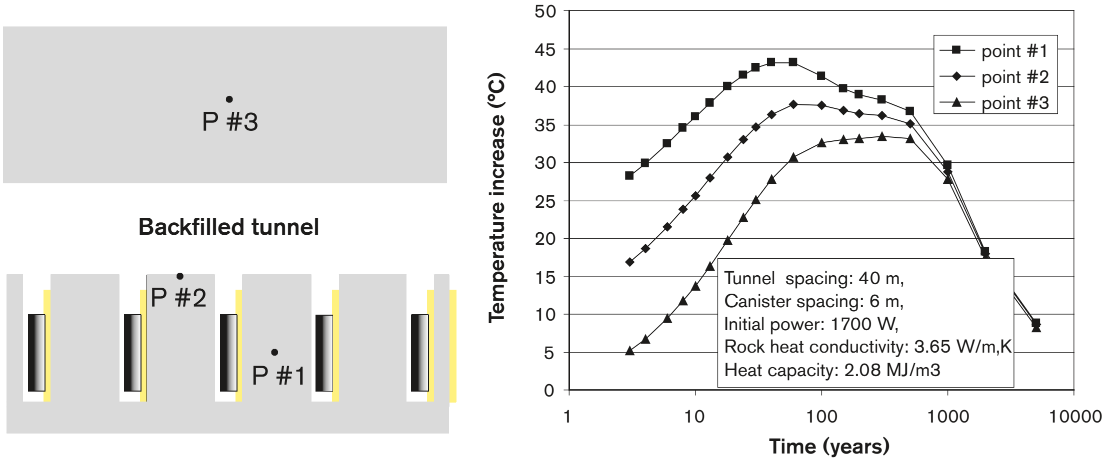


Figure 2-1. *Temperature increase at three points in the near field. The temperatures are calculated using an analytical solution derived by /Claesson and Probert 1996/. Absolute temperatures are obtained by adding the geothermal temperature. Here the repository is modelled as one large rectangular grid of canisters, whereas the real repository will be divided into a number of deposition areas separated by unheated corridors along the transport tunnels. This simplification makes very little difference to calculated temperatures and does not have any influence until after a few hundred years.*

2.1.7 Handling in the safety assessment SR-Site

Excavation/operation period

In the safety assessment, all canisters are assumed to be deposited simultaneously although, in reality, deposition will be distributed over time. For the near field of a given canister, the only effect of distributing over time is to offset the local thermal timescale. For confirmation, the thermal evolution in the near field of an individual canister was modelled assuming deposition to take place at different rates (one canister every second day and one canister every 4th day) /Hökmark et al. 2009/. Provided that this is done systematically, i.e. deposition area by deposition area, without allowing very long periods of time to elapse between deposition in neighbouring tunnels, the deposition sequence is of no importance to the temperature evolution of the individual canister. This low sensitivity to details in the deposition pattern is the basis for the assumption of simultaneous deposition of all canisters made, for instance, in the site engineering report /SKB 2009d/ and the reason for neglecting heat transport during the excavation/operation period.

Temperate climate domain

The temperatures at the walls of the deposition holes and in the buffer are calculated as a part of the thermal modelling performed specifically to establish the canister spacing in the site engineering reports such that the temperature limit (100°C in the buffer) is not exceeded for any canister position. Additional calculations are performed in /Hökmark et al. 2010/ to find how the buffer peak temperature varies among the canister positions because of the spatial variability in heat transport properties in the two Forsmark rock domains. In addition, the process is modelled in thermo-mechanical near-field and far-field analyses to assess thermally induced stress changes and deformations /Hökmark et al. 2010/.

Models; The thermal models are described in /Hökmark et al. 2009/.

Boundary conditions; There are two boundary conditions: the time-dependent heat flux from the deposition holes and the constant temperature at the cooled ground surface.

Handling of variables influencing the process; All variables considered to influence the process (Section 2.1.2), except for the temperature, are included in the models either directly (repository geometry) or indirectly (matrix mineral composition).

Handling of variables influenced by the process; The temperature is a model output.

Periglacial- and glacial climate domain

During the one million year assessment period, several glacial cycles with permafrost and glacial conditions are likely to occur in Sweden. However, major changes to colder climates are not expected during the first 1,000 years after repository closure, meaning that these changes are not relevant for the determination of peak temperatures in the repository. Rather, the safety related issue for colder future conditions relates to freezing of the rock, with the possible subsequent freezing of the backfill and the buffer, which might affect the canister and the host rock.

The development of permafrost is determined by the same relationships as those governing the thermal evolution in the host rock for temperate conditions, described above, see also Section 2.2.

The calculation of permafrost depth is rather straightforward by analytical or numerical models, if the thermal properties of the rock, the geothermal heat flow and the surface conditions (temperature, snow/ice coverage, etc) over time are known. Of these factors, the dominant uncertainties are related to the surface conditions, whereas the geothermal heat flow and the thermal conductivity of the rock are rather well-known. The detailed handling of the heat-transport process for periglacial- and glacial conditions in SR-Site is therefore described in the SR-Site Climate report, Section 3.4 /SKB 2010c/.

Earthquakes

Heat transport is not an issue for the induction of earthquakes, nor is it substantially modified by the occurrence of earthquakes.

2.1.8 Uncertainties

Uncertainties in mechanistic understanding

Heat transfer from the deposition holes, through the geosphere and across the ground surface is a relatively uncomplicated process. The process description is based on fundamental physical laws without conceptual uncertainties.

Model simplification uncertainties in SR-Site

The main model simplification is to regard the heat transport in the geosphere as determined solely by linear heat conduction. The uncertainties associated with this simplification are small. Non-linearity (temperature dependence of the rock heat conductivity) may correspond to an error of between 0.5°C and 1°C in the peak buffer temperature if this dependence is not explicitly accounted for /Hökmark et al. 2009/. Neglecting convection is pessimistic and has small effects /Thunvik and Braester 1991/.

Input data and data uncertainties in SR-Site

Input data used in the calculations are compiled and discussed in the SR-Site data report /SKB 2010b/.

The nature of the data uncertainty associated with rock heat temperature calculations in general and peak buffer temperature calculations in particular is described in /Hökmark et al. 2009/ along with typical uncertainty ranges of the different input parameters. The actual margins used to account for the uncertainties in the peak buffer temperature calculations made to establish the canister spacing in the different rock domains are given in the site engineering reports /SKB 2009d, e/.

2.1.9 Adequacy of references supporting the handling in SR-Site

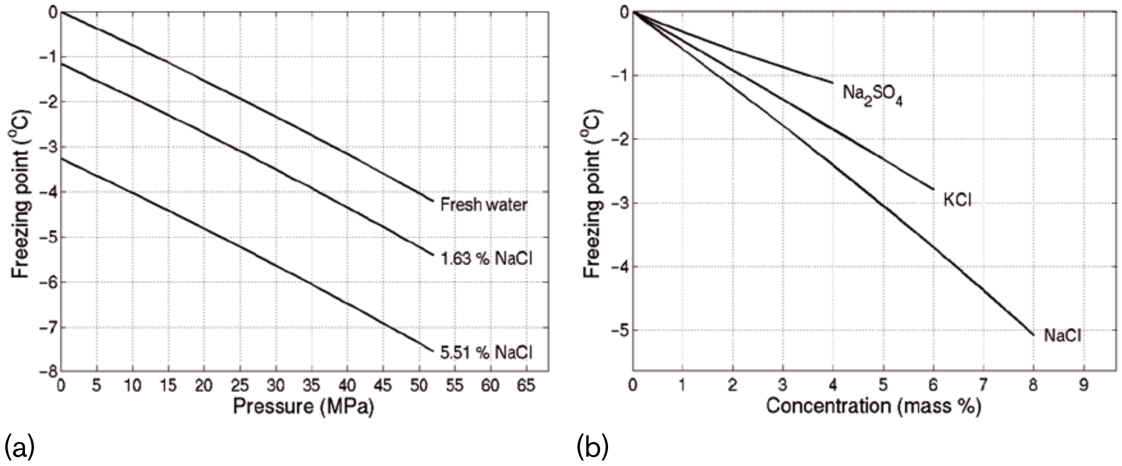
The supporting references /Hökmark et al. 2009/, /Hökmark et al. 2010/ and /SKB 2009d/ are SKB reports that have undergone a documented factual- and quality review.

2.2 Freezing

2.2.1 Overview/general description

Fresh water in the geosphere freezes under atmospheric pressure (101.325 kPa) at a temperature of 0°C. The freezing process is primarily governed by the temperature, but also by groundwater pressure, composition of the groundwater and the adsorptive capacity of ground matter. The freezing point of fresh water and saline (NaCl) water is lowered with increasing pressure by approximately 0.08°C/MPa in the pressure range 0.1–50 MPa, as depicted in Figure 2-2a, and with increasing salinity concentration, as shown in Figure 2-2b. The adsorptive capacity of the ground matter depends mainly on the physical properties and the specific surface area of minerals in the porous medium. The larger the adsorptive capacity, the lower the temperature required to freeze a certain amount of water.

Freezing of groundwater is an integral part of the physical processes occurring in the geosphere under cold climates and has a direct or indirect impact on its thermal, hydrochemical and mechanical behaviour. Heat transfer is influenced through the thermal properties of the frozen ground and by latent heat from the phase change. Since the conduction of heat is the main process that determines heat transfer in the geosphere /e.g. Hartikainen et al. 2010/, except in highly conductive fracture zones, the amount of freezing water dominates the rate of freezing and the depth to which freezing can extend. In principle, the larger the amount of freezing water, the lower the freezing rate. This results from the fact that the warming effect due to the latent heat overcomes the cooling effect due to the increased thermal diffusivity in the frozen ground. Freezing of water results in the ground becoming almost impermeable, which in cases of widespread permafrost strongly reduces the regional groundwater flow and changes the overall groundwater circulation /e.g. Hartikainen et al. 2010, Vidstrand et al. 2010a/. Exclusion of salts can occur during the freezing of saline groundwater, leading to a redistribution of the salinity concentration around the freezing front /Hartikainen et al. 2010/ (see also Section 5.12). The freezing of *in situ* water leads to a volume increase of approxi-



(a) (b)

Figure 2-2. *(a) Pressure-freezing point diagrams for fresh water from /CRC 1998/ and for NaCl aqueous solutions of concentrations of 1.63 and 5.51 weight-% from /Guignon et al. 2005/. (b) Concentration-temperature phase diagrams at normal atmospheric pressure for NaCl, KCl and Na_2SO_4 aqueous solutions from /CRC 1998/.*

mately 9% when going from liquid to solid state. This volume increase causes expansion of porous matter and of fracture openings, hence affecting the mechanical (effective) stress state. Moreover, especially in sedimentary units but also in fracture fillings, the gradual freezing of adsorbed water over a sub-zero temperature range can induce movement of moisture from the unfrozen ground to the freezing zone for ice formation. This can enhance the deformation of the ground and result in the widening of fractures. Freezing, when it takes place cyclically with thawing, can result in frost cracking and breakdown of the ground, increasing the overall rate of weathering and degradation of the ground /Williams and Smith 1989, Yershov 1998, French 2007/.

2.2.2 Dependencies between process and geosphere variables

Table 2-2 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 2.2.7.

Table 2-2. Direct dependencies between the process "Freezing" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes.	Periglacial Glacial	Temperature from model calculations of heat transport (Section 2.1).	Yes. Through the release of latent heat in the freezing process.	Periglacial Glacial	Included in permafrost models.
Groundwater flow	Yes. But mainly in highly conductive fractures with large flow.	Periglacial Glacial	Included in 2D permafrost model	Yes.	Periglacial Glacial	Included in 2D permafrost model. See also Section 3.1 Groundwater flow.
Groundwater pressure	Yes.	Periglacial Glacial	Included in permafrost models.	Yes. By partial freezing of water in the pore space under overburden pressure.	Periglacial Glacial	Included in permafrost models.
Gas phase flow	Yes. But only in highly conductive fractures with large groundwater flow.	Periglacial Glacial	Neglected; little significance.	Yes.	Periglacial Glacial	See Section 3.2 Gas flow/dissolution.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Repository geometry	No. But indirectly through heat transport and temperature.	–	–	No.	–	–
Fracture geometry	Yes. The amount of freezing water is related to fracture geometry.	Periglacial Glacial	Continuum porous medium models adopted. Detailed fracture geometry neglected; low-porosity rocks.	Yes. By volume increase going from liquid to solid state.	Periglacial Glacial	Neglected, little significance.
Rock stresses	No. But indirectly through fracture geometry and groundwater pressure.	–	–	No. But indirectly through fracture geometry.	–	–
Matrix minerals	No. But indirectly through thermal properties affecting heat transport and temperature.	–	–	No.	–	–
Fracture minerals	Yes. Affects water adsorption capacity.	Periglacial Glacial	Neglected; little significance compared with other influences.	No.	–	–
Groundwater composition	Yes.	Periglacial Glacial	Use of site-specific groundwater salinities in modelling studies.	Yes. By exclusion of salt.	Periglacial Glacial	Included in 2D permafrost modelling. See also Sections 5.12 and 3.2.
Gas composition	Yes. But only when vapour-ice phase change occurs.	Periglacial Glacial	Neglected; little significance.	Yes. But only when vapour-ice phase change occurs.	Periglacial Glacial	Neglected; little significance.
Structural and stray materials	No. But indirectly through their thermal properties and impact on groundwater composition.	–	–	Yes. But only if freezing occurs at repository depth.	Periglacial Glacial	Neglected; assumptions made regarding grout properties in different applications, see Section 5.8.
Saturation	Yes. Affects the amount of freezing water.	Periglacial Glacial	Neglected; saturated conditions in the bedrock is assumed.	Yes. Degree of saturation decreases.	Periglacial Glacial	Neglected; saturated conditions in the bedrock is assumed.

Temperature in bedrock; The temperature is the main variable that governs the process. The temperature at which freezing occurs is dependent on the pressure and composition of groundwater, and on the adsorptive capacity of the pore space.

Groundwater flow; Groundwater flow, when sufficiently large to contribute to the heat transport, will influence the freezing process. In highly conductive fracture zones freezing can be reduced considerably. Freezing of water in the fractures decreases the hydraulic conductivity to a very large extent, by about 4–6 orders of magnitude. This significantly reduces regional and local groundwater flow and indirectly has an effect on the overall groundwater flow pattern.

Groundwater pressure; An increase in the groundwater pressure decreases the freezing point. On the other hand, the groundwater pressure is affected by the amount of freezing water in the pore space, the mechanical properties of the ground matter and the effective stress state of the rock.

Gas phase flow; Gas flow can influence the vapour-ice phase change, just as groundwater flow does in freezing. Also, the decreased permeability of frozen ground reduces the local and regional gas flow, and indirectly affects the overall gas flow pattern.

Repository geometry; The repository geometry does not have any direct influence on the freezing process, but the heat from the repository counteracts the downward propagation of the freezing front /Hartikainen et al. 2010/.

Fracture geometry; The amount of freezing water and the adsorptive properties of the porous medium depend on the fracture geometry. In fractures with varying aperture (in effect all fractures) wider parts may freeze while narrow parts remain unfrozen unless temperature is lowered further.

Freezing can have some influence on the fracture geometry at shallow depths due to the frost cracking. Close to the surface frost wedges can be formed to the depth of some metres. Otherwise, there can be widening of fractures due to freezing but the effect is probably reversible as thawing takes place.

Rock stresses; Effective rock stresses can influence the groundwater pressure through changes in the rock pore volume and vice versa.

Matrix minerals; The process will not influence the mineral composition of the rock matrix. The mineral composition of the individual rock types is important for the rock thermal conductivity and for the rock heat capacity, and hence for the rate of freezing and propagation of the freezing front.

Fracture minerals; The adsorptive capacity of the porous medium depends on the properties of fracture minerals. There are no studies that quantify or describe the style and scope of fracture mineral alterations that could take place as a result of freezing. However, it has been observed that the partial freezing of water can increase the chemical activity of the ground matter in cation exchange reactions between soil mineral particles and adsorbed water /Yershov 1998/.

Groundwater composition; The composition of the groundwater affects the freezing point in such a way that the freezing point is decreased with increasing concentration of compounds like dissolved salts. Exclusion of salts during freezing can lead to redistribution of groundwater composition /Hartikainen et al. 2010/ (see also Section 5.12).

Gas composition; The gas composition can influence the vapour-ice phase change and vice versa.

Structural and stray materials; Structural and stray materials can alter the chemical composition of groundwater, and can, therefore, have an indirect influence on the freezing point of water.

Saturation; The amount of freezing water is related to the degree of saturation. Moreover, because the thermal conductivity is lower in an unsaturated material, the freezing rate is changed.

2.2.3 Boundary conditions

Thermal boundary conditions

Since the thermal regime of the ground does not involve any heat sinks that can cool the ground temperature below 0°C, freezing of the soil and bedrock can only develop from the ground surface. Hence, a ground surface temperature below 0°C is required for freezing of groundwater. The ground surface temperature in turn is an outcome of heat exchanges across the boundary layers between the atmosphere and the ground /Lockwood 1979, Washburn 1979, Lunardini 1981, Williams and Smith 1989, Smith and Riseborough 1996, Yershov 1998/. Depending on the climatic conditions and the nature of these boundary layers, the inter-annual ground surface temperature can deviate from the air temperature in a range between approximately –1 and +8°C, which may be exemplified by air temperatures and modelled ground surface temperatures for Forsmark (Figure 2-3).

In winter, a surface temperature lower than the air temperature can result from a thin snow cover on a bare ground surface, whereas with a full vegetation cover and sufficient thickness of snow cover, the surface temperature can be considerably higher than the air temperature. However, the annual mean ground surface temperature is in general higher than that of the air. This means that a mean annual air temperature lower than between –1.5 and –9°C typically is required for perennial freezing of ground to take place.

Naturally, the ground temperature and hence the freezing of ground are also controlled by the geothermal heat flow from the Earth's interior and by the thermal characteristics of the bedrock. Although, geothermal heat flow is rather steady in time, it is to some extent affected by long-term

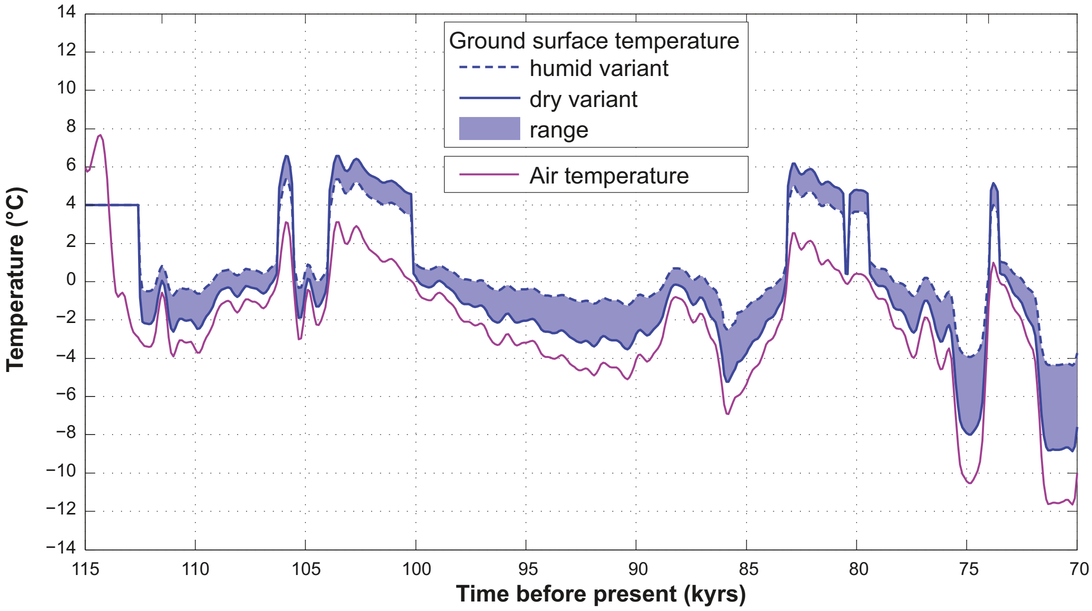


Figure 2-3. *Air temperature curve reconstructed for Forsmark for the first c. 45,000 years of the last glacial cycle and associated modelled ground surface temperatures for the location of the repository, used for permafrost modelling /Hartikainen et al. 2010/. The figure shows ground surface temperatures for one dry and one humid variant of climate development. Ground surface temperatures are several degrees warmer than the air temperature. Uncertainties in the air temperature curve are discussed in the SR-Site Climate report /SKB 2010c, Section 3.4.4 and Appendix 1/.*

climate-related variations at the Earth's surface, such as the waxing and waning of ice sheets. Geothermal heat flow has a large regional variation in Fennoscandia /Näslund et al. 2005/, which in turn have an effect on the development of perennial freezing of ground.

For the Forsmark site, the prevailing surface conditions, such as air temperature and surface cover (soil, vegetation, snow cover), are the main factors governing the spatial and temporal development of permafrost and perennially frozen ground. Subsurface conditions, such as bedrock thermal properties, geothermal heat flow, groundwater salinity and heat produced by the repository, modify the spatial and temporal permafrost development, but are of secondary importance compared with surface conditions /SKB 2010c, Hartikainen et al. 2010/.

Hydraulic boundary conditions

Hydraulic boundary conditions have a direct effect on the freezing process through the groundwater pressure which may lower the freezing point of the groundwater. The major hydraulic effects occur during periods of glacial conditions on the ground surface. An overlying ice sheet can increase the subglacial groundwater pressure in proportion to the ice-sheet thickness by up to about 30 MPa, in which case the freezing point can decrease sufficiently to keep the entire subglacial bedrock unfrozen /SKB 2010c/. A similar, but smaller, effect can occur when submarine perennially frozen ground is affected by the pressure of water bodies.

Furthermore, groundwater flow, carrying fresh glacial meltwater or saline seawater through the boundaries of the region of interest, can influence the freezing process indirectly by altering the groundwater composition.

Mechanical boundary conditions

Mechanical boundary conditions only have an indirect impact on the freezing process through the effective stresses.

2.2.4 Model studies/experimental studies

Relevant issues relating to freezing processes in the geosphere, based on literature reviews, have been reported by /Gascoyne 2000, Ahonen 2001, Vidstrand 2003, Vidstrand et al. 2010a/. Some recent experimental investigations of thermal, hydrochemical and mechanical impacts of freezing on bedrock properties have been reported by /Wegmann et al. 1998, Ruskeeniemi et al. 2002, Ruskeeniemi et al. 2004, Kleinberg and Griffin 2005/, whereas model studies dealing with permafrost development in ground under climate change can be found in e.g. /Lunardini 1995, Delisle 1998, Kukkonen and Šafanda 2001/. More recently, some model studies on thermo-hydro-mechanical impacts of freezing processes on bedrock properties with implications for interactions between glaciers and permafrost in a time frame of a glaciation cycle (~ 100,000 years) have been conducted, e.g. /Bauder et al. 2003, Hartikainen 2004, SKB 2006e, Person et al. 2007, Lemieux et al. 2008a, b, c, Hartikainen et al. 2010/. The effects of freezing of the geosphere on groundwater flow have been studied by e.g. /Vidstrand et al. 2010a/.

2.2.5 Natural analogues/observations in nature

Freezing of water in the geosphere is a common feature in Boreal and Arctic climates that occur in the temperate and periglacial climate domains described below. Surficial freezing processes can be observed at any locality in Sweden during winter. In addition, discontinuous alpine permafrost with perennially frozen ground has been estimated to occur down to 350 m depth in Swedish Lapland /Isaksen et al. 2001/, and the evidence of a cold surface layer e.g. /Pettersson et al. 2003/ indicates that perennially frozen ground exists also beneath parts of polythermal glaciers, i.e. glaciers that consists of ice both at and below the pressure melting point temperature. A full-scale field experiment on the growth of permafrost was conducted by /Mackay 1997/.

The present-day distribution of permafrost in the northern hemisphere is illustrated in Figure 2-4.

2.2.6 Time perspective

Due to natural fluctuations of insolation intensity in time, freezing of the ground can develop to a depth of a few centimetres on a daily basis to some metres on a yearly basis in a Boreal-Subarctic climate. Changes in ground surface temperature due to climate change can lead to development of permafrost and perennial freezing of the ground. If the mean annual ground surface temperature decreases from the present-day value to a value of below approximately –8 to –10°C, perennial freezing of ground can develop down to 400 m depth in the bedrock in a time frame of 100,000 years, as illustrated in Figure 2-5.

2.2.7 Handling in the safety assessment SR-Site

Temperate, periglacial and glacial climate domains

Development of permafrost and the depth of perennially frozen ground together with the evolution of ground temperature in a time frame of a glacial cycle, including temperate, periglacial and glacial climate domains /SKB 2010c/, are estimated by the use of 1D and 2D models. These are based on present day site-specific characteristics and initial conditions. For a reconstruction of permafrost development for the last glacial cycle, surface boundary conditions are produced by ice sheet- and global isostatic adjustment modelling. The conditions reconstructed for the last glacial cycle are subsequently used to construct a future reference glacial cycle, while colder surface boundary conditions are specified by modifying the reference glacial cycle conditions according to relevant climate cases, see SR-Site Climate report, Section 3.4 /SKB 2010c/.

Earthquakes

Not relevant.

2.2.8 Uncertainties

Uncertainties in mechanistic understanding

There are no major uncertainties in understanding of mechanistic processes regarding permafrost development. Minor uncertainties are associated with the fact that the geochemical weathering characteristics of the geosphere due to freezing and thawing processes are not yet well-founded.

Source:International Permafrost Association, 1998.
Circumpolar Active-Layer Permafrost System (CAPS), version 1.0.

Figure 2-4. Permafrost distribution in the Northern Hemisphere /UNEP/GRID-Arendal 2005/.

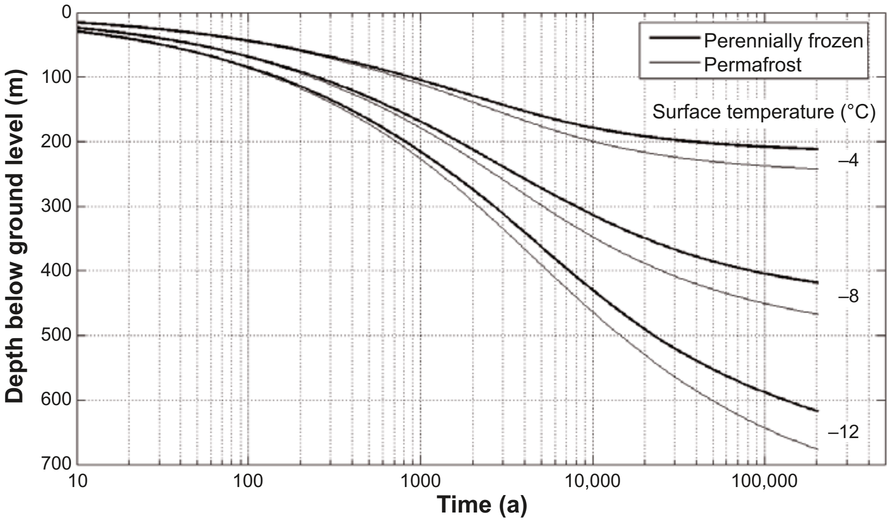


Figure 2-5. Evolution of permafrost (0°C-isotherm) depth and perennially frozen ground depth for constant ground surface temperatures of –4, –8 and –12°C at the Forsmark site with present-day mean characteristics, after /SKB 2010c/.

Model simplification uncertainties in SR-Site

Permafrost simulations have been performed in 1D and 2D. The 2D study constitutes a complement to the preceding 1D study, and they were made in order to investigate and illustrate the site specific spatial (along the profile) development of permafrost and frozen ground at Forsmark. The major model simplification in 1D permafrost modelling studies is the exclusion of lateral variations in physical properties, boundary conditions and geometry. For example, full consideration of the anisotropy of thermal conductivity and heat capacity and the features of water bodies and topography, as well as the heat generation from the spent fuel, requires 3D modelling. However, this is to a large extent taken care of by the 2D modelling study that has been performed /Hartikainen et al. 2010/. Minor uncertainties in the 1D modelling experiments are associated with the fact that the exclusion of salts in freezing of groundwater is not included. The process of freeze-out of salts is included in the 2D modelling.

The 1D modelling approach could, in certain situations, result in somewhat higher temperatures than would be calculated using a 2D or full 3D approach. In the context of permafrost development, the effect of groundwater flow, cooling down the bedrock, is the most important factor here. However, compared with heat conduction, groundwater flow has only has a minor role in permafrost development, as indicated by the 2D modelling results that included groundwater flow. Furthermore, the anisotropy of thermal properties is not a problem in 1D or 2D, since one can choose a combination of thermal properties that would give the lowest temperatures, or at least very close to the lowest temperatures. Therefore, it is unlikely that 3D simulations would yield notably lower temperatures than the range obtained by the full series of 1D and 2D sensitivity modelling studies that have been performed.

The 2D modelling approach used for studying talik formation has limitations since the important 3D groundwater flow network is missing /Hartikainen et al. 2010/. However, the limitations still allow for a first order study of talik formation in the Forsmark region.

Input data and data uncertainties in SR-Site

The reference glacial cycle surface boundary conditions, produced by the ice sheet- and glacial isostatic adjustment (GIA) models and used as input data for the permafrost simulations, constitute one example of a relevant, plausible future climate evolution. It is not a prediction of future climate, and therefore should not be associated with uncertainties in this respect. In order to cover the uncertainty in future climate, the reference evolution is accompanied by other possible future climate cases, together covering the full range of possible future climate variations within the time frame of a glacial cycle /SKB 2010c/.

Bedrock data

Some data uncertainty exists relating to thermal conductivity and heat capacity of rock at the Forsmark site /e.g. Sundberg et al. 2009/. In the calculation of ground temperature and the rate of freezing, thermal conductivity is the most important input parameter in terms of thermal properties of the ground /Hartikainen et al. 2010/. Some uncertainty also exists in determination of hydraulic and mechanical properties of bedrock and salinity concentrations of groundwater versus depth /SKB 2008a, 2009a/.

The *in situ* ground temperature has been measured in boreholes to a depth between 500 and 1,400 m. Between different boreholes the temperature at a specific depth varies in a range of 2°C /SKB 2005a, b, 2006a/. There is an uncertainty in the 1D permafrost study associated with determination of the *in situ* temperature and geothermal heat flow in the depth range of 1,000–10,000 m for the thermal boundary and initial conditions of the model. Based on the results and the investigations on ground temperature modelling by /Sundberg et al. 2009/, the uncertainty associated with determination of the ground surface temperature from the air temperature as well as with estimation of the *in situ* temperature and geothermal heat flow for the 1,000–10,000 m-depth for the thermal boundary and initial conditions of the model have been reduced considerably in the 2D permafrost modelling study.

The uncertainty in geothermal heat flow was investigated and described in /Sundberg et al. 2009/.

In general, the uncertainties in thermal characteristics of the bedrock and geothermal heat flow have a significantly smaller impact on modelled permafrost and freezing depths than uncertainties related to ground conditions and climate /Hartikainen et al. 2010/.

Surface conditions

As a complement to the 1D permafrost studies made for Forsmark /SKB 2006e, Sections 3.4 and 4.4.1/, the main objective of the 2D modelling study was to investigate impacts of surface conditions on the spatial (along the profile) development of permafrost and perennially frozen ground using site-specific information on climate and landscape features including water bodies and topography. An approach based on the Topographical Wetness Index (TWI) was introduced to describe the vegetation and snow cover in relation to the prevailing evolving climate and surface moisture conditions. TWI was used to identify and locate four relevant surface condition types, dry, moist-humid, wet and peatland, that could be expected to occur on the profile in Boreal-, Subarctic- and Arctic climate zones. Thereafter, ground surface temperatures were calculated from an air temperature curve by making use of n-factors that yield a statistical relation between the air and ground surface temperatures in consideration of climate and surface moisture conditions /Hartikainen et al. 2010/. Due to considerable uncertainties related to the description of surface conditions by TWI and modelling of ground surface temperatures by means of n-factors, two variants, one humid and one dry for reconstruction of last glacial cycle conditions and a severe permafrost case were analysed.

Temperature curve

Major uncertainties exist in the temperature curve used for the permafrost modelling, including uncertainties as to its representativity for the last glacial cycle climate as well as to its application to describe possible future climate cases. A detailed discussion and description of these uncertainties is found in /Hartikainen et al. 2010, Appendix 1/ and in the SR-Site Data report /SKB 2010b/. To cover the estimated uncertainties in air temperature curve reconstructed for the last glacial cycle, a large range of sensitivity cases and alternative variations of the temperature curve have been analysed. This was also motivated by the fact that the variation in surface conditions and climate has a larger impact on modelled permafrost and freezing depth than bedrock thermal conditions and geothermal heat flow.

2.2.9 Adequacy of references supporting the handling in SR-Site

The SKB reports produced for SR-Site that support the handling of the freezing process /Sundberg et al. 2009, SKB 2010c, Hartikainen et al. 2010/ have all undergone the SR-Site QA system handling, including a documented factual review procedure. Also the SR-Can Climate report /SKB 2006e/ and the site descriptions /SKB 2008a, 2009a/ have undergone a documented factual review. Other references used to support the handling of the freezing process are either books /Yershov 1998, CRC 1998/ or peer-reviewed papers from the scientific literature.

3 Hydraulic processes

3.1 Groundwater flow

3.1.1 Overview/general description

Groundwater

Groundwater is water found beneath the ground surface[1]. It is contained in voids in soils and rocks. At depth, the voids generally contain only groundwater – the subsurface is said to be saturated. Near the surface, there is generally a region where some of the voids contain air – the subsurface is said to be unsaturated. In the unsaturated region, the fraction of voids containing groundwater generally decreases with increasing elevation. However, there may be isolated saturated regions of so-called perched water within the unsaturated region. These result from variations in the rock properties.

Figure 3-1 shows a simplified schematic of the hydrologic cycle and the occurrence of subsurface and surface water. The water table, which is the level at which the pressure in the groundwater is atmospheric, is very close to the upper boundary of the saturated region. In the absence of perched water, the water table[2] is the level at which water is first encountered as an open borehole or well is drilled or excavated into the rocks. The water table is generally a subdued and smoothed version of surface topography, which comes to the surface at marshes, streams, rivers, lake margins and sea-coasts.

In fractured crystalline rock, the voids range in size from microscopic pores in the rock matrix to visible apertures in fractures and fissures. Groundwater flows predominantly in the void space of the interconnected fractures and this flow plays a key role in the performance of a repository for radioactive waste. In the event of radionuclide release from the repository, the groundwater flow and retention processes control the rate at which radionuclides move away from the repository and where they migrate; and groundwater chemistry is a key factor in determining the chemical environment of the repository, which potentially affects radionuclide migration and corrosion of materials within the repository.

The hydraulics of groundwater is described in many standard textbooks such as /Bear 1972, Freeze and Cherry 1979, de Marsily 1986, Domenico and Schwartz 1998/.

The hydrologic cycle

Groundwater forms part of the hydrologic cycle (Figure 3-2). In this cycle

- Water evaporates from seas, lakes, rivers, streams, marshes, soils and surfaces of vegetation, and is given off by plants (transpiration) to form water vapour in the atmosphere.
- Some of the water vapour in the atmosphere condenses to form water droplets. These may grow and eventually fall to the ground as rain, and some may freeze, falling to the ground as hail or snow.
- Some rainfall, and some water from melting snow and ice will run along the ground surface to nearby marshes, streams, rivers, lakes and seas (surface run-off), and some will infiltrate into the ground and flow down towards the water table.
- Some of the infiltrating water will be taken up by plants and may then be returned to the atmosphere by transpiration, and some may be absorbed into smaller pores in rocks and soils by capillary forces, leading to increased saturation.
- The remainder of the infiltrating water flows down to the water table, providing recharge for the groundwater system.

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[1] In groundwater hydrology, groundwater refers to the water in the saturated zone below the water table. However in drainage of agricultural lands, groundwater sometimes also refers to the water in the unsaturated zone above the water table. For simplicity and clarity of presentation, the term is used here for all water beneath the ground surface.

[2] Strictly speaking, in a rock in which groundwater flows predominantly through fractures, rather than referring to the water table, one should refer to the piezometric surface for the first flowing feature encountered, that is the level of the top of a column of water that could be supported by the pressure in the water first encountered, (This is because water might first be encountered below the water table in a fracture sloping up to the water table.) However, the term water table is used in this report for clarity.

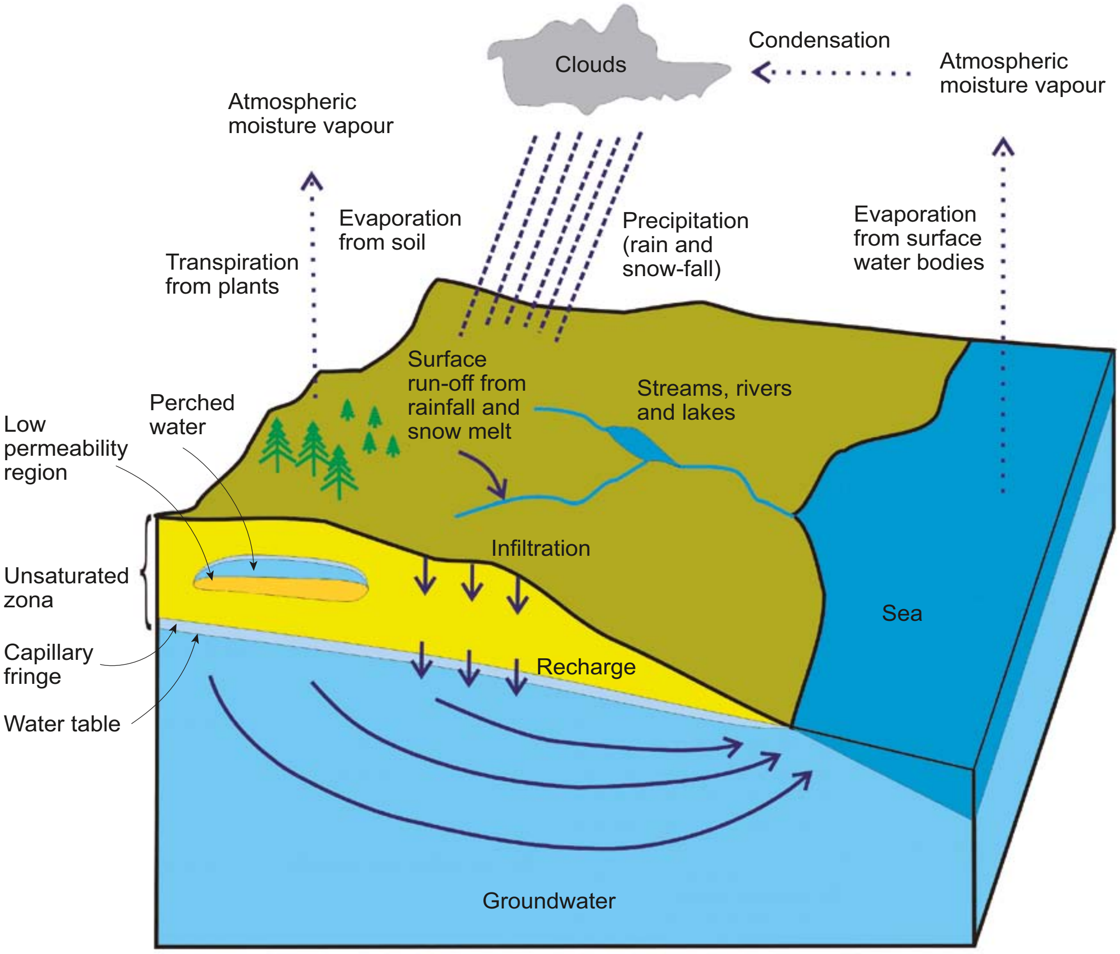

***Figure 3-1.** Simplified schematic of the hydrologic cycle and the occurrence of subsurface and surface water.*

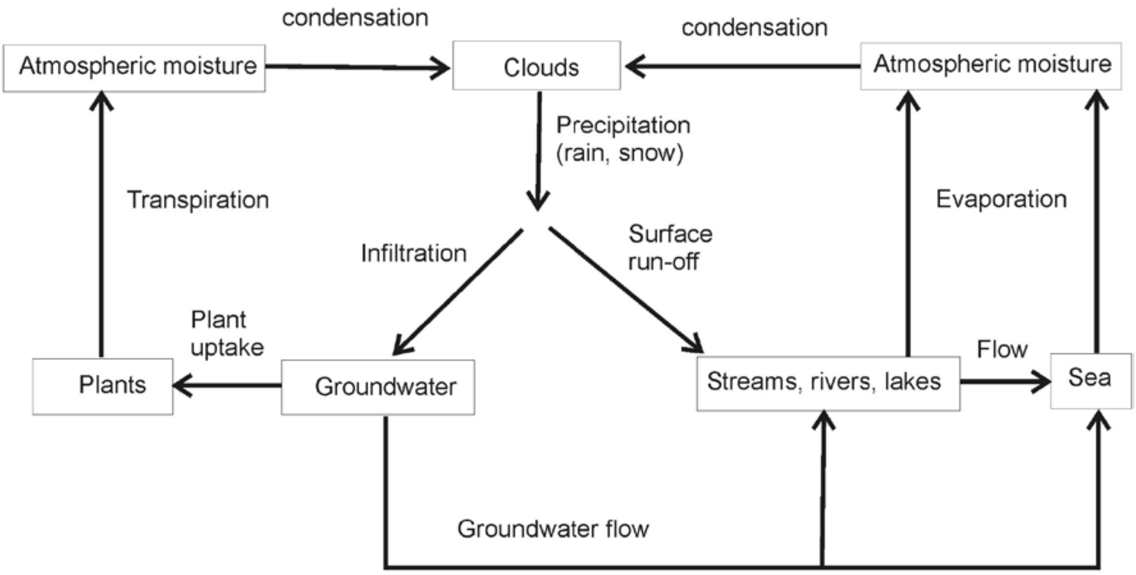

***Figure 3-2.** The hydrologic cycle in simplified form.*

Beneath the water table, groundwater flows through the ground, ultimately discharging where the water table comes to or above ground surface or the sea/lake bed (Figure 3-1). This will generally be at lows in the topography. It may also occur where rocks through which groundwater cannot flow readily come to the surface. The discharging water forms springs or contributes to marshes, streams, rivers, lakes or seas. Although surface water bodies generally correspond to regions of discharge from the groundwater system, in some circumstances there may also be recharge to the groundwater system beneath parts of rivers or lakes. This happens where the water table is below the level of the surface water body, which is being supplied with water by surface flows.

Flow patterns in Sweden

In Sweden, the water table is generally close to the ground surface. This is because precipitation generally is larger than evapotranspiration and because the permeability of the bedrock is often low. Consequently, groundwater tends to build up to elevations where it can be discharged as runoff within the surface hydrological systems (Figure 3-1).

Generally a groundwater flow system consists of local flow cells superimposed on the overall regional flow. The near-surface flows correspond to the local flows; the flow at depth corresponds to the regional flow system. In Sweden, because the water table is close to the ground surface and local topographic gradients are similar to or greater than the regional topographic gradients, the local flow cells tend to extend to greater depths than the expected depth of a repository. Thus, the flow at repository depths is generally determined by local flow cells, which largely depend on local conditions /Holmén et al. 2003, Follin and Svensson 2003/.

The simple pattern of groundwater flow linked to topography described above may be modified by the presence of large-scale structural features, such as fracture zones or faults. These may act as either flow conduits or barriers to flow, e.g. the Dolerite dykes at Laxemar, and result in flow cells with length scales controlled by the structural features rather than topography. For example, at Forsmark, the uppermost part of the bedrock is characterised by large horizontal fractures/sheet joints. This ‘shallow bedrock aquifer’ is nearly horizontal, extends over distances of several kilometres and is generally more transmissive than the surrounding rock, and so controls the groundwater head in its vicinity /Follin 2008, Follin et al. 2008, Follin et al. 2007/. It leads to the head varying more smoothly in the vicinity of the feature than would otherwise be the case, shielding the deeper rocks from the head variations corresponding to the detailed topographic variations. Due to the sparsity of fracturing at repository depth at Forsmark, /Joyce et al. 2010a/ found that groundwater pathways are often dominated by a single or small number of deformation zones, such the size of flow cells is controlled by the size and inter-connection of deformation zones. A strong structural control on pathways is also seen at Laxemar /Joyce et al. 2010b/.

Typically the groundwater salinity increases with depth, with a region of nearly fresh water near the ground surface, and brine at great depth. The salinity is also higher beneath the sea. The groundwater density increases with increasing salinity. If dense and light waters are present at the same elevation, the denser water will tend to flow beneath the lighter water and the lighter water will tend to flow above the denser water. Thus, fresh water will tend to flow up where it meets saline water beneath the sea, and discharge near the coast. Where waters of different salinity flow past one another, they will tend to mix (see also Section 5.2) because of hydrodynamic dispersion and diffusion. The mixing tends to reduce the density difference and hence the force driving flow.

As well as driving flow, density variations can also act to reduce flows. If the density depends only on elevation, decreasing with increasing elevation, then this acts to reduce the flow, possibly to very low levels. However, density increasing with increasing elevation is an unstable condition if the density gradient is large enough, and convection cells will form.

The temperature is not significantly affected by the groundwater flow but is predominantly controlled by conduction (see Section 2.1), except perhaps in the more permeable near-surface rocks, where advection may contribute to heat transport. The temperature increases with depth because of the flow of heat from the Earth’s core. The resulting geothermal gradient is usually fairly constant (because the thermal conductivity of the rocks does not vary greatly) and is about 15°C per kilometre, although there may be geothermal anomalies. The increased temperature at depth will tend to counter the effect of the increased salinity at depth on the density and viscosity.

The flow pattern outlined above would be modified by the construction, operation and subsequent presence of a deep repository (see Section 3.1.4).

Influence of gas flow

Groundwater normally contains dissolved gases (mainly nitrogen and helium in Sweden). The gas in solution has negligible effect on the groundwater properties. However, if the pressure of the groundwater is reduced, dissolved gas may come out of solution, for example, as groundwater flows towards a repository tunnel where the pressure would be considerably lower than the normal groundwater pressure at that depth. This would lead to a region of two-phase (gas-water) flow. In this region, the rock would effectively become less permeable to groundwater, which would affect the groundwater flow during the excavation and operation periods. Additional gas may enter the rock pores and fractures immediately adjacent to the repository during excavation and operation.

The repository will also be a potential source of gas (see Section 3.2). The gas might be produced as free gas, which would have effects similar to those indicated above, or it might dissolve in the groundwater as it was produced, in which case it would have negligible impact on the groundwater flow. Overall, the quantity of gas that would be produced is likely to be small.

Influence of climate-related conditions

The current groundwater flow system is significantly affected by past climate-related conditions and cannot be fully understood unless these are considered. The last major ice sheet retreated from Sweden about 13,000 to 8,000 years ago. The presence of an ice sheet and its basal conditions significantly alters the groundwater flow regime. The waxing and waning of ice sheets also affect the global sea level, and isostatic depression and rebound occurs in the vicinity of an ice sheet. Together these factors will cause shoreline migration and the boundary conditions for groundwater flow will change, as the land is submerged beneath the sea and vice versa. In periods of cold climate and beneath cold-based ice sheets, permafrost and frozen ground may develop.

The climate-related conditions that have prevailed in the past and that can be expected in Sweden in a 100,000 year time perspective are described in the SR-Site Climate report /SKB 2010c/. Based on issues and processes of importance for repository safety, three *climate domains* have been defined for which characteristic climatically determined environments prevail. These are the *temperate, periglacial* and *glacial domains* /SKB 2010c/. To these climate domains can be added periods when the land is submerged. The conditions for groundwater flow within each domain are fully described in /SKB 2010c/ and are summarised below.

During periods of temperate conditions, the main factor of importance for groundwater flow is shoreline migration. It is assumed that the precipitation over a year in Sweden always will be larger than the evapotranspiration, and that the formation of deep groundwater always is large enough for the groundwater table to follow the topography. When an area is transformed from being covered by the sea, or a lake, to land, groundwater flow will change from being driven by density to being driven by topography, and areas of discharge can be transformed to recharge areas. These dynamic boundary conditions influence the large-scale flow pattern, and some flow arises in the deep-lying saline groundwater /Voss and Andersson 1993, SKB 2008a, 2009a/.

Periods of temperate domain are typical of interglacials, but also occur during the warmer phases of a glacial. During the early phases of an interglacial, a fast fall of shorelines can be expected due to high rates of glacial rebound. During later phases of an interglacial, the increase in global sea levels will cause rising shorelines in areas where the isostatic depression is limited. In areas where the isostatic depression is large, the fall of shorelines will continue at a successively slower rate. During glacials, the shoreline of the contemporary Baltic is determined by the ice-sheet extent and the relative shoreline at its connections to the sea (see further /SKB 2010c/). Likewise, its salinity is also determined by its connections to the sea, such that it may exist as a freshwater lake rather than a marine or brackish sea.

During periods of permafrost, the main factor of importance for groundwater flow is the extent of frozen ground. Depending on climate conditions, permafrost may develop only in exposed areas, e.g. north slopes, or everywhere beneath the land surface. Even during severe climate conditions, permafrost will not develop beneath larger water bodies. Regions of unfrozen ground (taliks) may therefore be found, and may link the deep groundwater flow system to surface recharge and discharge.

As the water freezes in the formation of permafrost, exclusion of salt occurs. This may give rise to a zone of increased salinity beneath the advancing freezing front (see Sections 2.2 and 5.12).

Frozen ground can be regarded as impermeable, and the presence of permafrost and a seasonally frozen active layer restricts the infiltration of water and its recharge to groundwater systems. Compared with the temperate domain, precipitation can be expected to decrease significantly. However, due to the cold climate conditions and the abundance of water during the summer season it is still expected to exceed evapotranspiration and the groundwater table is expected to follow the topography in unfrozen areas. The presence of frozen ground will also change locations of recharge and discharge and drive groundwater flow to greater depth. In the vicinity of unfrozen areas, potential gradients may be high. The periglacial climate domain and the development of permafrost is further described in the Climate report /SKB 2010c/.

During periods of glacial conditions, groundwater flow will be determined by the presence of the ice sheet and its hydrological systems. If the ice sheet is cold based with permafrost beneath the ice and no liquid water is present at the ice/bed interface, groundwater flow can be regarded as stagnant. If the ice sheet is warm based, melt water is generated at the ice/bed interface. In areas near the front of the ice sheet, precipitation and melt water from the ice surface can be transported to the bed through moulins and crevasses. The conditions for groundwater flow will be determined by the configuration of the sub-glacial hydrological system of the ice sheet, which can be either a fast or slow flow system. A fast system transmits large quantities of water at low pressure and can be thought of as a tunnel system. A slow system transmits smaller quantities of water while maintaining a higher pressure and holding larger volumes of water. An example of a slow system is a linked cavity system. Ice-sheet hydrology is further described in the SR-Site Climate report, Section 3.2 /SKB 2010c/.

The presence of an ice sheet will also alter rock stresses and, especially under a warm-based ice sheet, high water pressures can be expected. The altered stress state will affect fractures and fracture apertures. Fractures may grow and it is even possible that new fractures may form (see Sections 4.3 and 4.4). Thus, the conductive features of the bedrock can be expected to be altered during the different phases of ice-sheet advance and retreat.

The growth and retreat of ice sheets may also lead to considerable redistribution of Quaternary deposits and to the creation of new deposits. This would change the particular pattern of the deposits, but their properties would be expected to remain within their current ranges. Although the changes would have considerable impact on the flows in the Quaternary deposits themselves, they would not be expected to have much impact on the deep groundwater flow.

Influence by humans

Future human actions may impact on the groundwater flow system. Groundwater abstraction from a borehole will change the flow field in the vicinity of the borehole, and lower the water table locally. The effects can extend for some distance from the borehole, if it is drilled into a major permeable fracture zone, which is usually attempted (in order to be able to abstract as much water as possible). If a repository is located within the zone of influence of a water-abstraction borehole (taking into account the effects of intersected fracture zones), then the flow through the repository may be affected by the abstraction. Groundwater abstraction from a borehole may also change the distribution of salinity. For example, there may be saline upconing beneath an abstraction borehole. Changes in the salinity distribution will affect the groundwater flow locally.

Even if a groundwater abstraction borehole is located too far from a repository to affect the flow through the repository, it may affect potential flow paths to or from the repository. Indeed, if an abstraction borehole is downstream of a repository, it may be the discharge location for some of the groundwater flowing through the repository.

Vaults, tunnels and shafts are likely to have a similar, but larger effect on groundwater flow than water abstraction from boreholes. Unless the bedrock walls are completely sealed, water will leak in to the vaults, tunnels or shafts and must be pumped out to prevent them from getting water filled.

Other human actions, such as construction of dams, drainage systems, urbanisation, and abstraction of water from streams, rivers and lakes can also lead to changes in groundwater recharge or discharge. Activities that may impact groundwater flow are further discussed in the SR-Site FHA report /SKB 2010f/.

Modelling of groundwater flow

Driving forces

Groundwater flow is driven by the forces of gravity and the mass times acceleration of the groundwater due to gradients in pressure. The flow is proportional to the gradient of the sum of pressure and gravitational potential, and to the ability of the rocks to carry groundwater – that is, how permeable the rocks are – and inversely proportional to the groundwater viscosity. The gravitational force is proportional to the groundwater density.

Groundwater properties

For conditions relevant to a spent fuel repository, the groundwater viscosity and density are determined almost entirely by the salinity (a measure of the total concentration of dissolved solutes) and temperature of the groundwater. Although, in principle, the viscosity and density are also affected by the pressure, in modelling for a repository in Swedish bedrock, the effect of the pressure, which is small, only needs to be taken into account implicitly in the specific storage (see below).

The viscosity decreases with increasing temperature, and increases with increasing salinity, both of which typically increase with depth. For example, at a typical repository depth of about 500 m the temperature in Swedish bedrock would be about 7°C higher than the surface temperature, and at a depth of about 2 km the temperature would be about 30°C higher than the surface temperature. The latter temperature difference would lead to the viscosity at such a depth being about half the value at the surface. The viscosity would also be affected (in the opposite direction) by the increased salinity at such a depth. The density increases with increasing salinity. As a function of temperature, the density of fresh water has a maximum at 4°C.

Groundwater flow models

There are two main types of groundwater flow models: continuous porous medium (CPM) models and discrete fracture network (DFN) models. (There are also other types of models, such as channel models, which are used occasionally.) In practice, the models are implemented numerically, using, for example, finite-element or finite-difference methods. There are many programs that can be used for CPM modelling and a small number of programs that can be used for DFN modelling. There are also a very small number of programs that can be used to carry out modelling in which CPM and DFN representations are used for different parts of the domain of interest. In the SKB programme, the computer code ConnectFlow /Hartley and Holton 2004/ is used for such hybrid modelling.

CPM groundwater flow models treat the rocks through which the groundwater flows as a continuum characterised by quantities defined at all points in a 3D region. In contrast, DFN models explicitly model the fractures through which groundwater flows in some rocks, and are characterised by quantities associated with the fractures (and generally not by quantities associated with the intervening rock matrix). CPM models are considered the appropriate models for certain types of rock in which flow is predominantly through an interconnected network of pores in the rock matrix, such as many sandstones, or for soils and unconsolidated deposits. In other rocks, such as the fractured crystalline rocks in Sweden, groundwater flows predominantly through fractures. For such rocks, DFN models represent more of the hydraulic characteristics of the rock, such as water moving through discrete features, as is considered to be the case physically, and further the models attempt to represent some of the details of fracture geometry, size, connectivity and openings. Nevertheless, the overall flow on suitable length scales (longer than those of the fractures) can be modelled (to a good approximation) using CPM models /La Pointe et al. 1995, Jackson et al. 2000, Svensson and Ferry 2004/. In the SKB programme, heterogeneous CPM models that represent fractured rocks are referred to as Equivalent Continuous Porous Medium (ECPM) models.

CPM models

Groundwater flow can be represented using CPM models of varying levels of complexity, as appropriate to different circumstances. All the models are based on Darcy's law, which relates the specific discharge $\mathbf{q}$ (the volumetric flowrate of groundwater through unit area, $m \cdot s^{-1}$) to the driving force. Darcy's law (for saturated flow) is:

$$\mathbf{q} = -\frac{k}{\mu}(\nabla P - \rho \mathbf{g}) \tag{3-1}$$

Where

$\mathbf{q}$ is the specific discharge (also known as the Darcy flux) (m·s^{-1})

k is the permeability of the rocks (m^2)

μ is the viscosity of the groundwater (Pa·s)

ρ is the density of the groundwater (kg·m^{-3})

P is the pressure in the groundwater (Pa)

$\mathbf{g}$ is the acceleration vector due to gravity (m·s^{-2})

The permeability is a function of the geometry of voids within the rocks. It depends on the number density of the pores, their connectivity and their dimensions. The contribution to the permeability from a pore is of the order of a high power of its diameter or aperture, so smaller pores contribute relatively little to the permeability. The permeability is a tensor, that is, varies by direction. It addition, it is usually also heterogeneous, that is, varies from point to point, typically over several orders of magnitude.

Near open boreholes and tunnels, the specific discharge is generally less than that predicted by Darcy's law. This is because there is an additional resistance to flow above the viscous drag which corresponds to Darcy's law. This additional resistance is due to inertial effects at high fluxes, and to turbulence at very high fluxes /Scheidegger 1956, de Marsily 1986/. The specific discharge may also be less than that predicted by Darcy's law in compacted clays due to disturbance of the clay particles leading to a closing of coarse pores or increases of tortuosity.

Constant-density flow

The simplest CPM model for groundwater flow is that in which variations in salinity and temperature can be neglected (sometimes referred to as constant-density flow). The corresponding flow equations comprise Darcy's law together with the equation for conservation of mass. In this case, Darcy's law can be written in simpler form in terms of the hydraulic head h (m):

$$h = \frac{P}{\rho g} + z \tag{3-2}$$

where z is vertical elevation (m) and g is the magnitude of gravity. Then Darcy's law becomes

$$\mathbf{q} = - K \nabla h \tag{3-3}$$

introducing the hydraulic conductivity (m·s^{-1})

$$K = -\frac{k \rho g}{\mu} \tag{3-4}$$

The particular form for the mass conservation equation depends on the assumptions made. A suitable expression for this case (allowing for compressibility of the rock in the vertical direction) is

$$\frac{S_s}{g}\frac{\partial P}{\partial t} - C\frac{\partial \sigma}{\partial t} + \nabla \cdot (\rho \mathbf{q}) = 0 \tag{3-5}$$

where

S_s is the specific storage of the rocks, which depends on the compressibilities of the rocks and the groundwater (m^{-1})

C is a coefficient related to the compressibility for the rocks (m^{-2}·s^2)

σ is the overburden stress (Pa).

The first term on the left-hand side of Equation (3-5) represents the effect of the compressibility of the water and the pore space. If the pressure in the water is reduced then the water expands, and also the pore space decreases in volume. The result is that water flows out of the pore space.

For completeness, the second term on the left-hand side of Equation (3-5) has been included, although it is often omitted. This term represents the effects of changes in the overburden stress. In most groundwater flow modelling, this term does not contribute, because the overburden stress does not change significantly. However, in modelling flow over geological timescales it may be necessary to include this term. For example, the overburden stress will be changed significantly by the presence of a thick ice sheet during glacial periods. If the overburden stress is accompanied by a corresponding increase in liquid pressure at the ground surface, however, the stress term has little influence /Lönnqvist and Hökmark 2010, Hökmark et al. 2010/.

Unsaturated flow

Flow in the unsaturated zone above the water table is described by modified versions of the above equations. Because the groundwater is only present in some of the pores, the rest being filled with air (or other gases) the permeability of the rock is reduced. This can be characterised in terms of the relative permeability: the ratio of the permeability to that if all the pores were water-filled. This is taken to be a function of the saturation (the fraction of the pore space that is filled with groundwater). The relative permeability usually exhibits hysteresis: its value depends on the history of the saturation, for example whether the rock is drying or wetting. In practice, hysteresis is seldom modelled. This type of approach is used in ConnectFlow /Hartley and Holton 2004/.

The saturation is taken to be a function of the water pressure (often called pore pressure). This is because the pores drain as the pressure decreases below atmospheric pressure. The wider pores tend to drain first because the capillary forces that hold water in the pores are smaller for wider pores. However, the particular pores that drain will depend on the way in which the pores are connected. Water may be held in some of the wider pores because it cannot drain through narrow bottle-necks because of capillary forces. Again, the relationship between the water pressure and the saturation exhibits hysteresis, although this is seldom modelled in practice.

The relations between the relative permeability and the saturation and between the saturation and the pore pressure are called constitutive relations. Many forms for such relations have been proposed for different media, but the usual forms probably do not give good representations for unsaturated flow in fractured rocks.

An alternative approach is to perform saturated groundwater flow calculations below a free surface which is located where the calculated pressure is atmospheric. Depending on the particular implementation, either boundary conditions are applied at the free surface or horizontal flows are neglected above it. The location of the free surface and groundwater flow are then calculated iteratively. DarcyTools /Svensson and Ferry 2004/ uses a version of this approach.

The unsaturated zone does not have much effect on the long-term performance of a deep repository in Sweden, because it is typically very thin compared to the expected depth of a repository. However, during the construction of a repository the water table will be drawn downward, probably leading to an unsaturated zone of several metres or tens of metres above the repository (modelling of the excavation and operation phases at Forsmark /Svensson and Follin 2010a/ estimate maximum draw-downs around 10 metres depending on grouting efficiency). This will take some time to resaturate after repository closure.

The unsaturated flow equations can also be used to describe the resaturation of the backfill in the repository, and the equations are related to the two-phase flow model used to represent gas migration from a repository (see Section 3.2).

Variable-density flow

The model outlined above can be extended to account for changes in density and viscosity due to variations in salinity and temperature. It is necessary to represent the density and viscosity as appropriate functions of salinity and temperature. Functions that provide good representations of measured data over much wider ranges of temperature and pressure than those of interest in a performance assessment for a deep repository have been developed by various authors, and are compared in /Adams and Bachu 2002/.

It is also necessary to determine the way in which the salinity and temperature vary over the region and times considered. The salinity is determined by the concentrations of the constituents dissolved in the groundwater. These constituents are transported by the flowing groundwater by advection, dispersion and diffusion. (Dispersion is discussed further in Section 5.2.) Some of the constituents may also interact with the minerals on the surfaces of the pores and fractures through which the groundwater is flowing.

In cases in which the flow is through a fractured rock, represented by a CPM model, solutes dissolved in the groundwater may also diffuse into and out of relatively immobile groundwater in the rock matrix between the fractures carrying the bulk flow – the process of rock-matrix diffusion. (Transport of the groundwater constituents is similar to the transport of radionuclides by the flowing groundwater, see Section 6.1, except that radionuclide concentrations are so low that they have negligible effect on the density and viscosity, and that the groundwater constituents generally do not decay but may interact with minerals on the surface of the pore space.)

Until recent years, modelling of variable-salinity groundwater flow considered only the transport of the overall salinity. However, recently, various studies have been carried out in which the transport of several groundwater constituents has been considered /Rhén and Smellie 2003, Hartley et al. 2005a, b/ and a capability for carrying out such calculations has been implemented in the ConnectFlow program. Such calculations facilitate comparisons with experimental measurements of groundwater composition (in order to test models). However, transport calculations for several groundwater constituents are more resource intensive computationally than calculations that address only the transport of salinity.

The simplest model for the transport of several groundwater constituents takes all the constituents to be conservative (i.e. non reactive and non-sorbing) and non-decaying, and further takes the diffusion-dispersion term in the transport equation for a constituent to be proportional to the concentration gradient for that constituent. The latter is an approximation, because in a multi-component system the diffusive term at least should be a linear combination of the concentration gradients of all the constituents (see for example, /Bird et al. 1960/), and this is probably also true for the dispersion term. With these approximations, the transport equations for a groundwater constituent in a CPM model for fractured rock taking rock-matrix diffusion into account are /Hoch and Jackson 2004/.

$$\frac{\partial(\phi\rho C_i)}{\partial t} + \nabla\cdot(\rho\mathbf{q}C_i) = \nabla\cdot(\phi\rho D\nabla C_i) - 2\omega D_e \left.\frac{\partial C_i'}{\partial w}\right|_{w=0} \tag{3-6}$$

$$\frac{\partial(\phi'\rho C_i')}{\partial t} = D_e \frac{\partial^2 C_i'}{\partial w^2} \tag{3-7}$$

where:

ϕ is the flowing porosity of the rocks (i.e. the fraction that constitutes voids, or fractures, through which groundwater is flowing) (–)

C_i is the mass fraction of the constituent (–)

D is the dispersion tensor ($m^2 \cdot s^{-1}$)

ω specific surface of the fractures per unit volume of rock (so 2ω is the flow-wetted surface per unit volume of rock) (m^{-1})

ϕ' is the matrix porosity of the rocks

D_e is the effective diffusion coefficient for the rock matrix ($m^2 \cdot s^{-1}$)

C_i' is the mass fraction of the constituent in the immobile water in the rock matrix (–)

w is a coordinate within the rock matrix (m).

The overall mass conservation equation in this case is

$$\frac{\partial(\phi\rho)}{\partial t} - C\frac{\partial(\sigma)}{\partial t} + \nabla\cdot(\rho\mathbf{q}) = 0 \tag{3-8}$$

For this model, any linear combination of the groundwater constituents satisfies the same transport equation. It is, therefore, possible to choose linear combinations that can be interpreted as the fractions of selected reference waters. This may be useful in presenting the results of flow calculations, and it facilitates comparison with experimental measurements of groundwater composition, which, in the SKB site investigation programme, have been expressed in terms of mixtures of certain reference waters /Laaksoharju et al. 2008b/.

The temperature of the rocks and groundwater is determined by the transport of heat through the rocks. Although some heat is transported by flowing groundwater by advection and dispersion like a groundwater constituent, the dominant process for heat transport is conduction through the rock matrix except in highly permeable rocks, (which in Sweden are usually only present near the ground surface). The model usually used to represent heat transport is

$$(\rho_a c_a)\frac{\partial(\theta)}{\partial t} + \nabla\cdot(\rho c_p \mathbf{q}\theta) = \nabla\cdot(\Gamma\nabla\theta) + \nabla\cdot(\phi\rho D\nabla\theta) \qquad (3\text{-}9)$$

where

θ is the temperature of the rock (and groundwater) (K)

ρ_a is the average density of the rock and groundwater (kg·m^{-3})

c_a is the average specific heat of the rock and groundwater (J·kg^{-1}K^{-1})

c_p is the specific heat of the groundwater (J·kg^{-1}K^{-1})

Γ is the thermal conductivity of the rock (W·m^{-1}K^{-1}).

The second term on the left-hand side of Equation (3-9) represents the effects of advection, and the second term on the right-hand side represents the effects of dispersion, which results from advection. As noted above, these terms can be neglected in many cases.

Other coupled processes

The discussion above addresses the transport of groundwater, heat and concentration (of a groundwater constituent) due to the relevant primary driving forces, which are the gradient of pressure minus hydrostatic pressure, the gradient of temperature and the gradient of concentration, respectively. On general thermodynamic grounds, it would be expected that each driving force would lead to transport of groundwater, heat and concentration (see for example, /de Marsily 1986, Scheidegger 1956/). For example, a temperature gradient would drive solute migration (the Soret effect), a concentration gradient would drive heat transport (the Dufour effect) and a concentration gradient would drive fluid transport (osmosis). However, the magnitudes of these processes are usually much smaller than the transport of a quantity due to its primary driving force, and are therefore not considered further here.

DFN models

DFN models explicitly represent fractures through which groundwater is flowing. In these models, there is no flow through the rock matrix between the fractures, although some models may represent diffusion of solutes (such as radionuclides or groundwater constituents) into effectively immobile groundwater in micro-fractures and pores within the matrix. DFN models provide more detailed and more realistic models for rocks, such as the crystalline basement rocks in Sweden, in which groundwater flows predominantly through fractures.

DFN models are implemented numerically. The equations for a DFN model consist of flow equations for each fracture, together with continuity of pressure and conservation of mass at fracture intersections. The fractures are idealised as 2D planar objects of simple shape, such as rectangles or circular discs. The mathematical flow equation for each fracture is a 2D analogue of the 3D CPM flow equations with the hydraulic conductivity replaced by the transmissivity. These equations are usually solved numerically using finite-element techniques, for example.

The behaviour of groundwater flow in a DFN model depends on the transmissivities of the fractures in the model and the way in which they are connected. Usually the properties of the fractures in a region of interest are not fully known. Therefore, a stochastic modelling approach is adopted. The number density of the fractures and the distributions of the fracture properties (orientation, size and transmissivity) are measured (or inferred from measurements). Then numerical realisations (or examples) of the fractures in the domain are set up in which the properties of the fractures in the numerical model are sampled statistically from the inferred distributions, so that the distributions of the fracture properties in the model reproduce the inferred distributions (to the extent possible). Observed fractures may also be modelled deterministically, that is represented explicitly in the model.

Multi-scale modelling

In practice, modelling groundwater flow for a repository performance assessment is likely to involve a number of models on different length scales. It is likely that detailed modelling on the scale of waste containers, or even smaller, will be needed in the vicinity of the repository to give the desired accuracy. However, calculations with a model that is this detailed everywhere and covers a domain extending to the boundaries of the relevant regional flow are unlikely to be practicable. This is because the number of finite elements (or grid blocks) would be too large. Whatever program is used, there are practical limits on the number of finite-elements in a numerical model because of the finite computer resources (memory and file storage) available, and from the need for the calculations to be completed in reasonable times (typically within a few days).

Therefore, it is likely that a combination of models on different scales, which separately contain a number of grid blocks near the limits for practicable calculations, will be used. Typically regional models extend over distances of tens or hundreds of kilometres, whereas a local model may extend over distances of a few kilometres, or less. Repository scale or near field models covering the rock surrounding several or several hundred deposition holes may also be required. The boundary conditions for the regional model will be determined from the relevant physical processes (such as the positions of regional water divides), whereas the boundary conditions for the local models will be obtained from the results of the calculations for the regional model. Even though the regional and local models may have similar numbers of grid blocks, the discretisation of a local model will be finer, because the domain is smaller, and so the local model can provide greater detail than the regional model in the region it covers.

Typically, a regional model might extend over distances of tens or hundreds of kilometres, whereas a local model may extend over distances of a few kilometres, or less. A regional model is likely to be a CPM model. In such a model, a CPM representation would be used both for rocks in which the groundwater flows through pores in the rock matrix and for those in which it flows through fractures. The model would include explicit representations of the larger features (such as regional faults) in the region of interest, though not the smaller features (such as individual fractures). The model can include a representation of the repository. It can also include a locally refined region in the immediate vicinity of the repository.

In Sweden, the host rock for a repository is likely to be one in which groundwater flows predominantly through fractures. (This is the case at Forsmark and Laxemar, for example.) Therefore, local DFN models are likely to be used. Local CPM models, in which the fractured rock is represented by an equivalent CPM (ECPM), can also be used. The local models will include representations of the larger features that cross the region modelled, together with smaller features (which it is not practicable to include in a regional model). Local DFN models may include a sub-region in the immediate vicinity of the repository in which smaller features than those that can be represented over the whole domain of the local model are modelled. Local models will generally include representations of the repository. Either ECPM and DFN representations, or a combination, may be used for this.

It is possible that models on different scales may be embedded, that is a model on one scale may directly include a model on a different scale. This avoids the need to transfer boundary conditions between different models, and ensures that the effective boundary conditions on the smaller model are consistent with the larger model, without iterating between the different models.

The multi-scale modelling approach outlined above may be extended further, through the use of even smaller-scale models of portions of a repository.

ECPM models

In the SKB programme, two kinds of heterogeneous CPM models, or Equivalent Continuous Porous Medium (ECPM) models, are used to represent groundwater flow through fractured rocks. ECPM models require values of the permeability tensor for the grid blocks. These values may be obtained from the underlying fracture network by a process known as upscaling.

The computer code ConnectFlow /Hartley and Holton 2004/ includes an ECPM approach where the flow through a block containing fractures is calculated for a given pressure difference across the block in a given direction. The equivalent permeability for the block is then the permeability tensor of a homogeneous block that would give the same overall flow through the block in different flow directions. Hence, the equivalent permeability tensor represents the flow capacity of the fractures within the block.

In the computer code DarcyTools /Svensson and Ferry 2004/, the equivalent permeability tensor is obtained by a slightly different upscaling approach to that described above. DarcyTools uses a staggered grid approach, with grid blocks associated with flow in a given direction centred on the corresponding faces of grid blocks associated with the pressure. Only large-scale features and fractures larger than a certain minimum size are taken to contribute to the equivalent permeability. The contribution from a fracture to the hydraulic conductivity in a particular direction is essentially given by the transmissivity of the fracture multiplied by the fracture length and width in that direction and divided by the volume of the grid block. Rock permeability is related to hydraulic conductivity by Equation (3-4). This process generally leads to an equivalent permeability field that is anisotropic and heterogeneous, noting that the fractions of grid blocks associated with flow in different directions are different.

Properties of the rocks affecting flow (the 'permeability' and fracture transmissivity)

The transmissivity of a fracture in a DFN model is analogous to the hydraulic conductivity times the thickness of a formation in a CPM model. It depends primarily on the fracture aperture, being proportional to the cube of the aperture in a simple parallel-plate model. (Hence the range of variations in transmissivity is much greater than the range of variations in aperture.) The transmissivity is also affected by the roughness of the fracture surfaces, and can be reduced by the presence of fracture fill. The transmissivity generally varies considerably (by several orders of magnitude) between fractures and even over an individual fracture. Because of the variation in transmissivity within a fracture, groundwater flow through a fracture will tend to follow a number of channels. These channels may change if the flow direction changes.

The connectivity of the fractures depends on their shape, distributions of size and orientation, distribution in space and the nature of fracture intersections and terminations. In many cases, the fractures can be categorised in terms of sets with particular orientation distributions.

There may also be extensive regions – fracture zones – with much greater fracture intensity than the surrounding rock. Fracture zones may have thickness of tens of centimetres to tens of metres and may extend for tens of metres to many kilometres. It is likely that there will be considerable variability within a zone. The transition between a fracture zone and the surrounding rock may be diffuse. That is, between the rock surrounding the fracture zone and the more intensily fractured core of the zone, there may be a region with an intermediate degree of fracturing. Fracture zones may provide the dominant flow paths for groundwater.

The transmissivity of a fracture may change over time, either as a result of changes in the effective stress or because of precipitation or dissolution of minerals within the fracture. The effective stress on a fracture is the difference between the total rock stress acting normally to the fracture and the fluid pressure in the fracture. At depth, it is dominated by the stress in the rock. Over time this may change. The main processes leading to stress changes on the timescales of interest are the temperature changes due to the heat given out by a repository and the load resulting from the presence of ice sheets during glacial periods /Hökmark et al. 2010/. The stress may also change because of tectonic changes (which are very slow), earthquakes, and as a result of the construction of a repository.

If there is a change in the effective normal stress, the fracture aperture and the fracture transmissivity will change in a way that depends on the properties of the two fracture surfaces. An increase in normal stress would tend to reduce the fracture aperture and may reduce the overall transmissivity depending on the distribution of contacts between the fracture surfaces and any filling material. Generally, the sensitivity of fracture transmissivity to stress changes is larger for fractures in low compression than for fractures in high compression. If the shear stress at the fracture surface increases, the opposite surfaces of the fracture will tend to move relative to one another. This might increase or decrease the fracture aperture and hence the transmissivity.

Changes to the stress within the rocks may also lead to existing fractures extending, to the reactivation of fractures that have become sealed, or even to the creation of new fractures (see Sections 4.3 and 4.4). The relative increase in fracture area per unit of rock mass volume that would follow from changes in the fracture geometry, caused by fracture propagation or fracture generation, is very small for the load evolution projected for the repository host rock /Hökmark et al. 2010/. Fracture apertures and hence transmissivities may also change over time as a result of rock creep (see Section 4.5).

The process of constructing the tunnels of a repository will tend to alter the properties of the rock in the immediate vicinity of the tunnels. The stress in a radial direction relative to the tunnel will be reduced, but the stress in a tangential direction will be increased. As a result, some fractures may close, decreasing their transmissivity and some may open, increasing their transmissivity, and there may be slip along some fractures. The behaviour of a fracture will depend on its orientation relative to the change in the stress field. An excavation damaged zone (EDZ) may also be created in the immediate vicinity of a tunnel, particularly if the tunnels are constructed using drill and blast techniques /SKB 2010l/. In the EDZ, additional fractures may be created and existing fractures may grow and/or change their aperture, leading to changes in transmissivity.

As well as the properties of the disturbed rocks around the repository, the properties of the tunnels (and shafts) of the repository may also affect the groundwater flow. However, the tunnels would be backfilled before repository closure and seals would be placed at selected locations within the tunnels. Provided that these backfillings and seals remain effective, they should prevent the tunnels acting as connected paths for flow over their whole length.

Precipitation of minerals within a fracture will reduce its aperture. The fracture may remain open, but with an aperture that is everywhere reduced, or open parts of the fracture may become blocked. Either way, the effect is to reduce the transmissivity of the fracture. Dissolution of minerals within a fracture will generally increase its aperture, leading to an increased transmissivity. However, it is possible that contact points between the opposite surfaces may dissolve and the fracture may then tend to close up under the prevailing stress. The porosity of the rock matrix, which affects the flow through its impact on rock-matrix diffusion of salinity, may also be affected by precipitation and dissolution.

3.1.2 Dependencies between process and geosphere variables

Table 3-1 shows the interactions of the process groundwater flow with the key variables that characterise the state of the geosphere. The handling in SR-Site is also indicated in the table and further described in Section 3.1.7.

Table 3-1. Direct dependencies between the process "Groundwater flow" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Temperature in bedrock	Yes. Affects viscosity, which affects flow. Affects also density, which may lead to buoyancy forces driving flow.	Excavation/ operation/ resaturation	Neglected; little significance compared with effects of drawdown and inflow to the repository.	Yes. But minor. In principle, heat is transported by flowing groundwater, as well as by conduction through the rock. However, the former is only significant in highly permeable rocks.	Excavation/ operation/ resaturation	Neglected; the effect is small.
		Temperate	Effect of geothermal gradient on density and viscosity considered in main calculations. Impact of thermal effects from waste addressed in scoping calculations for SR-Can /Hartley et al. 2006a/. Effect negligible and so not considered for SR-Site.		Temperate	Neglected in the main calculations; the effect is small. Effect allowed for in the scoping calculations of the impact of the heat from the waste carried out for SR-Can, but effect negligible /Hartley et al. 2006a/.
		Periglacial	Effect of geothermal gradient taken into account. Constant temperature distribution in time because effect of variations over time secondary to effect of permafrost.		Periglacial	Neglected; the effect is small.
		Glacial	Neglected; secondary to effect of ice sheet.		Glacial	Neglected; the effect is small.
Groundwater flow						
Groundwater pressure	Yes. Pressure gradient is one driving force for groundwater flow.	All	Included in the model.	Yes. Pressure and flow are coupled.	All	Determined from groundwater flow calculations.
Gas phase flow	Yes. Groundwater flow and gas flow are coupled.	Excavation/ operation/ resaturation	Effect of the gas phase taken into account implicitly for the excavation/operation phase using a model that represents the water table by a free surface. This can give the drawdown and inflow. Note that no gas is generated by the repository in this period. Effect of the gas phase taken into account explicitly in resaturation calculations using a simplified model of gas and water phase flow.	Yes. Groundwater flow and gas flow are coupled.	Excavation/ operation/ resaturation	Not explicitly modelled because drawdown and inflows can be determined from a model with the water table treated as a free surface. Gas phase flow not explicitly represented in resaturation calculations using simplified model.
		Temperate	Neglected in main flow calculations; small volume of gas generated and effects localised. Impact of gas assessed by scoping calculations for SR-Can /Hartley et al. 2006a/.		Temperate	Considered in estimates of the capacity for transport of dissolved gas carried out for SR-Can /Hartley et al. 2006a/. See Section 3.2 Gas flow/dissolution.
		Periglacial	Neglected; effect secondary to effect of permafrost.		Periglacial	Neglected; gas flow is a relatively minor process.
		Glacial	Neglected; secondary to effect of ice sheet.		Glacial	Neglected; gas flow is a relatively minor process.

Variable	**Variable influence on process**			**Process influence on variable**		
	Influence present? **(Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence** **(How/If not – Why)**	**Influence present?** **(Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence** **(How/If not – Why)**
Repository geometry	Yes. Repository geometry affects distribution and characteristics of flow paths.	Excavation/ operation/ resaturation	A detailed representation of repository tunnels included in model.	No. Does not change repository geometry.	–	–
		Temperate	A detailed representation of repository tunnels included in local flow model.			
		Periglacial	Neglected; effect secondary to other effects addressed.			
		Glacial	Neglected; secondary to other effects addressed.			
Fracture geometry	Yes. The fracture aperture, geometry and connectivity determine how permeable the rock is. The geometry of the pore space in the matrix will affect rock matrix diffusion, which may affect the groundwater composition (in particular the salinity) and hence the flow.	Excavation/ operation/ resaturation	Site-specific descriptions of geometry of fractures and fracture zones.	No. But indirectly through changes in groundwater composition affecting rock-water interactions. Also indirectly through changes to fracture apertures as a result of changes in groundwater pressure associated with groundwater flow, and possibly also glaciation	–	Indirect changes resulting from precipitation/dissolution not addressed because they are expected to be long-term and relatively very small. The changes to fracture aperture as a result of groundwater flow are not considered because they are considered to be small. The effect of possible high pore pressure beneath an ice sheet and 'hydraulic jacking' of fractures are addressed, see Section 4.3.7
		Temperate	Site-specific descriptions of geometry of fractures and fracture zones. Impact of EDZ addressed by assigning elevated hydraulic conductivity relative to the host rock. Changes over time neglected; small and within the uncertainties.			
		Periglacial Glacial	Continuum models based on site-specific descriptions of geometry of fractures and fracture zones.			
Rock stresses	No. But indirectly through changes in fracture geometry.		Neglected. However the effects of the changes in the rock stresses during repository excavation operation and resaturation on the properties of the fractures in the vicinity of the repository taken into account through modelling of the EDZ. Stress changes are expected to be relatively small, apart from changes due to repository construction, thermal fluxes from the spent fuel, ice-loading, tectonic changes at very long times and earthquakes.	No. But groundwater flow affects rock stresses indirectly through the contribution of the groundwater pressure to the effective stress. However, the changes in groundwater pressure are generally so small as to have negligible effect on the rock stresses, except for repository desaturation and resaturation and possibly ice-loading.		Neglected. Because effect generally small.
Matrix minerals	No. But indirectly through groundwater composition and diffusion out through the rock matrix.		Neglected; little significance compared with other influences considered.	No. But indirectly through matrix diffusion from flowing groundwater.	–	See chemical processes in Chapter 5.
Fracture minerals	No. But indirectly by affecting fracture geometry.		Neglected; little significance compared with other influences considered.	No. But indirectly through groundwater composition.	–	See chemical processes in Chapter 5

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Groundwater composition	Yes. Groundwater salinity affects its density and viscosity.	Excavation/ operation/ resaturation	Site-specific salinity effects considered.	Yes. Also affected by dispersion/ diffusion and matrix diffusion.	Excavation/ operation/ resaturation	Transport of salinity by advection and matrix diffusion is modelled.
		Temperate	Site-specific variations in and distribution of salinity and reference waters accounted for in the models.		Temperate	Transport of salinity and reference waters by advection and matrix diffusion is modelled.
		Periglacial Glacial	Site-specific salinity effects considered.		Periglacial Glaciation	Transport of salinity by advection and matrix diffusion is modelled.
Gas composition	No.	–	–	Yes. Dissolved gases transported by flowing groundwater may come out of solution where the pressure falls.	All.	Neglected; concentrations of dissolved gases are generally low.
Structural and stray materials	Yes. Grouting is likely to affect the flow.	Excavation/ operation/ resaturation	Sensitivity study in which permeability of nearby rock is reduced to simulate different levels of grouting.	Yes. Flow can affect degradation of grout locally.	Excavation/ operation/ resaturation	Neglected; see Section 5.8 Degradation of grout.
		Temperate	Grouting is, pessimistically, not represented.		Temperate	Neglected; see Section 5.8.
		Periglacial Glacial	Pessimistically neglected.		Periglacial Glacial	Neglected; see Section 5.8.
Saturation	Yes. Affects the effective permeability and thus flow.	Excavation/ operation/ resaturation	The effect of the changing saturation taken into account through models in which the unsaturated flow is handled in a simplified manner and in the region above the water table which in turn is represented is represented as a free surface (see Section 3.1.7). Addressed in calculations of flow in near-surface regions.	Yes. May change saturation.	Excavation/ operation/ resaturation	Modelled at the level of the ground being saturated or the water not present. Modelled in calculations of flow in near-surface regions.
		Temperate	Neglected. Unsaturated zone near surface has little effect on flow in deep rocks, which are saturated. Unsaturated zone taken into account in MIKE SHE calculations used to determine maximum potential recharge (precipitation less evapotranspiration).		Temperate	Neglected. Unsaturated zone near surface has little effect on flow in deep rocks, which are saturated. Unsaturated zone taken into account in MIKE SHE calculations used to determine maximum potential recharge (precipitation less evapotranspiration.
		Periglacial	Neglected; the ground would generally be saturated beneath the permafrost (unless a sufficiently large gas bubble forms).		Periglacial	Neglected; the ground would generally be saturated beneath the permafrost (unless a sufficiently large gas bubble forms).
		Glacial	Neglected; effects secondary to the effects of an ice sheet.		Glacial	Neglected; effects secondary to the effects of an ice sheet.

Temperature in the bedrock. In principle, groundwater flow affects temperature in the bedrock because heat is transported by flowing groundwater. However, the rocks at depth in Sweden have low permeability and low porosity, and so the heat transported by flowing groundwater is negligible in comparison with that transported by conduction through the rocks (see Section 2.1.1). The temperature in the bedrock affects the groundwater flow through the effect of temperature on the viscosity and density of the groundwater. The geothermal gradient leads to a variation of the viscosity with depth. (The temperature difference between the surface and the rocks at 2 km depth is about 30°C, which would lead to the viscosity being about half that at the surface. However this would be counteracted by the effects of salinity.) The geothermal gradient would also lead to the groundwater density decreasing with depth. The variations in the viscosity and density would affect the groundwater flow. The heat generated by the spent nuclear fuel would lead to a temperature perturbation that propagates out from the waste and ultimately falls off over time. The temperature perturbation would affect the groundwater viscosity and density, which would affect the groundwater flow. In particular, the variations in density would lead to buoyancy forces and convection cells would tend to form in the vicinity of the repository.

Groundwater pressure. Gradients in groundwater pressure provide one the forces driving groundwater flow.

Gas phase flow. If both gas and groundwater are present in the pores and fractures in the rock, the flows of gas and groundwater are coupled. In the unsaturated region extending down from the surface, it is not necessary to model the flow of gas because the pressure in the gas phase is very close to atmospheric because the gas is very mobile. Indeed, in most cases, it is adequate to treat the water table as a free surface.

Repository geometry. Groundwater flow does not affect the repository geometry. The repository geometry affects the flow because the backfilled tunnels and surrounding EDZ may provide permeable paths through the rocks and additional connections between the fractures.

Fracture geometry. Groundwater flow does not directly affect the fracture geometry. However, flowing groundwater may indirectly affect the fracture geometry through its effect on rock-water interactions and dissolution or precipitation of minerals within the fractures. (These effects occur on long time scales.) The fracture aperture, geometry, and connectivity are key properties that determine how permeable the rock is and so play a major role in determining the flow. The fracture geometry, and connectivity also define the matrix block geometry, which is a major control on rock-matrix diffusion. Rock matrix diffusion affects salinity and hence the groundwater density and viscosity, which are key fluid properties affecting the flow.

Rock stresses. Groundwater flow does not affect rock stresses directly, although it does affect pore pressure, which can alter rock stresses. For example, increases in pore pressure may generate effective stress reductions that possibly could lead to slip on critically oriented fractures. For pore pressure variations associated with saturation and desaturation of the repository host rock, the impact of that slip on stresses would be local and modest. Changes to the rock stresses would affect the properties of the fractures, in particular the aperture and hence transmissivity.

Matrix minerals. In principle, groundwater flow can indirectly affect matrix minerals, through its effect on the composition of groundwater flowing through the fractures which can affect the composition of the groundwater within the rock matrix and hence may lead to precipitation or dissolution of minerals within the matrix. However, these effects are considered to be small in relation to other processes. Also, in principle, matrix minerals can affect the groundwater flow through the precipitation or dissolution of minerals affecting the composition of groundwater in the rock matrix and diffusion of dissolved minerals out of the matrix affecting the composition and hence the density of the groundwater flowing in the fractures, which will affect the flow if the density changes are sufficiently large. However these effects are considered to be very small in relation to other processes.

Fracture minerals. In principle, groundwater flow can indirectly affect fracture minerals, through its effect on rock-water interactions and possible precipitation or dissolution of minerals. However, these effects are considered to be small in relation to other processes. Also, in principle, fracture minerals can affect the groundwater flow through the precipitation or dissolution of minerals affecting the composition and hence density of groundwater flowing in the fractures, which will affect the flow if the density changes are sufficiently large. However, these effects are considered to be small in relation to other processes. Dissolution and precipitation of fracture minerals is further described in Section 5.6.

Groundwater composition. Groundwater flow affects the groundwater composition through the transport of dissolved constituents of the groundwater. Advection, dispersion, diffusion and rock-matrix diffusion all contribute to the transport of these dissolved constituents. The groundwater composition affects the groundwater flow because the groundwater salinity, which is determined by the groundwater composition, affects the groundwater density and viscosity.

Gas composition. Groundwater flow affects the gas composition because flowing groundwater can transport dissolved gases, which may come out of solution where the pressure falls. However, the concentrations of dissolved gases are generally low. The gas composition has negligible effect on the groundwater flow, for the same reason.

Structural and stray materials. The groundwater flow could affect the degradation of grout used to seal flowing features in the vicinity of the tunnels. As the grout degraded over time the permeability of the grouted rock would increase. Grouting in the vicinity of the tunnels would reduce the permeability of the rocks locally and affect the groundwater. It is likely that grouting would be focused on transmissive features, and so the local flow would be significantly affected.

Saturation. Groundwater flow would affect the saturation. A change in the level of the water table as a result of groundwater flow would correspond to a change in saturation in the rocks through which the water table moves. The saturation affects the effective permeability and hence the flow. The main changes to the saturation would occur during the period of excavation/operation/resaturation. These changes are taken into account in models in which only the flow in the fully saturated region is represented, with the water table modelled as a free surface, whereas both unsaturated flow and resaturation are modelled through simplified concepts. In calculations of the flows in the temperate period, unsaturated conditions are generally neglected. In some calculations, the unsaturated region in Quaternary deposits near the ground surface is taken into account.

3.1.3 Boundary conditions

The groundwater flow in a region is determined by the initial conditions within the region at a specific time, the groundwater inflows/outflows or pressures on the boundaries of the region, the composition of inflowing/outflowing water, the temperature of the rock, and the magnitude of sinks (i.e. abstractions) (and possibly sources, although these are unlikely) within the region.

In practice, rather than a region being selected, and boundary conditions determined for it, the domain for the largest-scale (regional) model will be determined by locations where boundary conditions can be sensibly specified on physical grounds, or will have little impact in the regions of interest (Figure 3-3). Boundary conditions for smaller-scale models are then obtained from the results for the larger-scale model.

For the regional model, lateral boundaries onshore are often located at regional water divides (through which there is no flow). These are usually close to ridges in topography or major rivers. Lateral boundaries may also be located at discharge areas. Providing the offshore lateral boundary conditions are sufficiently far beyond where most groundwater discharge to the seabed occurs (i.e. beyond any low permeability confining sediments on the seabed), then hydraulic gradients should be very low at this boundary and hence a no flow condition is appropriate.

One advantage of positioning lateral boundaries such that a no flow boundary condition can be justified is that this condition is far simpler to implement than fixed head conditions when considering long-term transients processes such as sea level changes and post-glacial rebound.

The bottom of the regional model is taken to be at a considerable depth (well below a repository) and the boundary condition here is usually also taken to be no-flow. There are two reasons for this. Rocks at depth tend to be less permeable than those near the surface, so that the flows at depth are smaller than those near the surface. Also the groundwater at depth tends to be more saline than the near-surface water. This stratification tends to lead to low flows at depth. Therefore, a no-flow boundary condition is a reasonable approximation. In some circumstances, it may also be an adequate approximation to use a shallower model, with the bottom boundary in the transition zone between deep brines and shallower fresh water and a no-flow boundary condition on the bottom boundary. This might be appropriate for cases in which the distribution of the deep brines does not

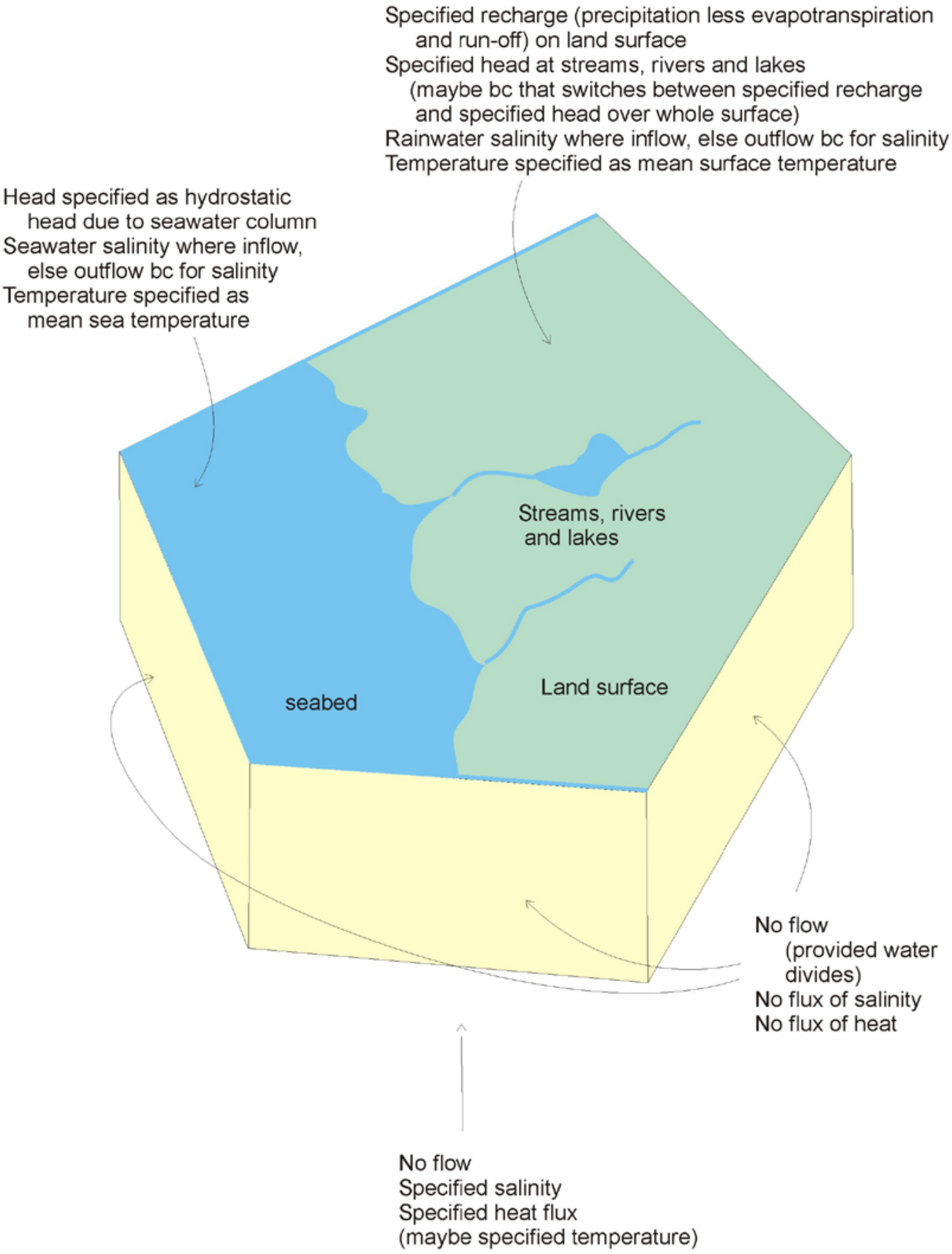

Figure 3-3. *Boundary conditions for a regional model.*

change greatly, for example, because the time period considered is short. However, if a case is considered in which the distribution of the deep brines may change, for example as a result of upconing, then it may be necessary to use a deeper model.

The top of the regional model is usually taken to be at approximately the topographic height of the land surface. Over most of the land surface there will be recharge to the groundwater system, and the physical boundary condition is that the recharge is specified. The value of recharge is average precipitation (including snow-melt) less surface run-off and actual evapotranspiration. Typically, recharge will be significantly less than precipitation, especially if the near-surface rocks are not very permeable.

It should be noted that modelling for a repository performance assessment considers timescales of many thousands of years. Day-to-day and seasonal fluctuations are of little interest (but may be important in characterising the near-surface hydrogeology), and it is only necessary to consider averages over times of order years. At onshore discharge locations (springs, marshes, streams, rivers, and lakes), that are connected hydraulically to the deep groundwater system, the physical boundary condition is that the groundwater head is at the level of the surface water. In practice, a numerical approximation that switches between the specified recharge and specified head boundary conditions as appropriate may be used. Offshore, the physical boundary condition is that the pressure at a location corresponds to the hydrostatic pressure of the column of sea-water at that location. This depends on the depth of the sea and its salinity.

In Sweden, the water table is generally close to the ground surface. Measurements of groundwater levels at Forsmark are within about 1m of ground surface in the Quaternary deposits and within about 5m of ground surface in the bedrock /Follin 2008/. Similarly, the depth to the water table at Laxemar is considered to be no more than a few metres /Werner et al. 2008/. Therefore, it is a reasonable approximation that the saturated flow takes place in the whole of the model, that is, to neglect the effect of the unsaturated zone, which is normally thin. However, it is necessary to consider the unsaturated zone in modelling groundwater flow during repository excavation and construction, since there is a potential for considerable drawdown of the water table in the vicinity of the repository. In reality, there are environmental requirements that the drawdown be limited by appropriate engineering measures, such as grouting during excavation and construction (the effects are examined in /Svensson and Follin 2010a/). Further, in the modelling of the temperate period (see /Joyce et al. 2010a/) a flux based boundary condition is specified on the top surface such that the simulated groundwater levels can be below ground surface, although unsaturated conditions are not imposed above the calculated water table. The actual boundary condition effectively switches between specified recharge where head is below ground surface and specified head where it is equal to above.

Over the land surface, recharging groundwater is generally almost fresh, and a reasonable physical boundary condition for salinity is that there is no flux of salinity where there is recharge. However, provided that the salinity in the near-surface region is low, the consequence of this boundary condition does not differ greatly from that for a boundary condition of zero salinity, which may be more convenient in numerical modelling. Where there is discharge onshore, the physical boundary condition is that the flux of salinity corresponds to the outflow of water at the calculated salinity. This boundary condition, which is sometimes called an outflow condition, also corresponds to the normal component of the dispersive/diffusive flux of salinity being zero. A reasonable boundary condition for the salinity at the bottom of the model is to prescribe the salinity on the basis of experimental observations of salinity at depth. Offshore, the physical boundary condition for salinity would be outflow of salinity where there is groundwater discharge, and the salinity of the sea water where there is inflow.

The physical boundary condition for temperature at the bottom of the model is a specified value of the heat flux from depth. In some circumstances, a suitable approximation to this may be to prescribe the temperature at the bottom of the model. At the top of the model, the physical boundary condition is a prescribed value of the temperature corresponding to mean annual ground surface temperature. This may differ slightly from the mean annual air temperature. For example, snow cover may insulate the ground from the air to some extent. In principle, the mean annual surface temperature varies slightly with elevation, and different values may be appropriate on land and offshore, but it may be a good approximation to take the values to be the same. The heat flux is generally almost vertical, and so an appropriate boundary condition on the lateral boundaries of the regional model is that there is no flux of heat through the boundaries.

The discussion above has addressed the boundary conditions for the most general models to be considered, which address groundwater flow, transport of groundwater constituents and heat transport. Simpler models may provide adequate approximations in some circumstances. Such models will use a subset of the boundary conditions discussed.

Over the timescale that will be considered in assessing the performance of a repository, the boundary conditions are transient for various reasons. For instance, changes in the surface elevation may affect the regions of recharge and discharge. The combined effect of the changing surface elevation and the changing sea level leads to the position of the shoreline changing, which will affect the location of some discharges.

The climate will change, which may lead to changes in recharge. The salinity of the sea may change. In glacial periods, recharge may be prevented because of the formation of permafrost. The position of permafrost would change over time. An ice sheet may be present at some times, and this would affect recharge. The appropriate physical boundary condition beneath the ice sheet may be a groundwater pressure corresponding to the pressure exerted by the ice sheet, or a specified recharge (allowing for loss to sub-glacial streams). Information about conditions beneath an ice sheet may be provided by ice-sheet models, see /Vidstrand et al. 2010a/ for a literature overview.

The discussion above has addressed the boundary conditions for regional models, which are decided on physical grounds. The boundary conditions for the smaller-scale models are usually the values of the groundwater pressure, salinity and temperature calculated in the regional model at the locations corresponding to the boundaries of the smaller-scale models. For some computer codes (e.g. ConnectFlow) it may be possible to nest models on different scales within a single combined model so that it is not necessary to explicitly transfer boundary conditions between different models, which greatly facilitates the modelling.

As well as boundary conditions, it is necessary to supply initial conditions for transient calculations. It is likely that there will be considerable uncertainty about aspects of the initial conditions for particular calculations. For example, the initial conditions for calculations of the evolution of the current groundwater flow system from the conditions after the last glacial period are not well known. The best that can be done is to postulate plausible conditions based on understanding of the system taking into account observations of, for example, groundwater chemistry.

In modelling the excavation, operation and resaturation of a repository, suitable boundary conditions on the wall of the tunnels are needed. During the excavation and operation periods, the groundwater pressure on the tunnel walls will be atmospheric. During the resaturation period, the pressure in the air remaining in the void space in the repository will slowly rise as it is compressed by incoming water. This would need to be modelled to provide an appropriate boundary condition.

3.1.4 Model studies/experimental studies

A large number of experimental studies have been conducted during the past 20 years at, among other places, the Stripa Mine /Fairhurst et al. 1993, Gnirk 1993, Gray 1993/, the Äspö HRL /Wikberg et al. 1991, Rhén et al. 1992, Emsley et al. 1997, Rhén et al. 1997/ and at Finnsjön in Sweden /Ahlbom and Tirén 1991, Ahlbom et al. 1992/. A number of important experimental studies have been conducted at Grimsel in Switzerland and at the Underground Research Laboratory, URL, in Canada as well. Modelling concepts have been tested and developed within SKB, and a number of international projects have been carried out such as Decovalex /Stephansson et al. 1996/, Intraval /Larsson et al. 1997/ and within the Task Force at the Äspö HRL /for example: Gustafson and Ström 1995, Svensson 1997a, b, Andersson et al. 2002a, b, Poteri et al. 2002, Winberg et al. 2003, Rhén and Smellie 2003/.

Additional insight concerning recharge and discharge patterns for groundwater flow has been gained in more recent modelling studies /Holmén et al. 2003, Follin and Svensson 2003, Ericsson et al. 2006, Ericsson and Holmén 2010/. These studies, performed for northern Uppland and eastern Småland, respectively, show that local flow cells can dominate groundwater flow at a typical repository depth. The flow cell dimensions are determined by the relation between local and regional gradients. Local gradients are effectively largely determined by the local topography. Thus, it is important to resolve the local topography in sufficient detail in numerical models.

The influence of extensive horizontal fractures/sheet joints in the uppermost bedrock at Forsmark in flattening heads above the repository region were investigated in /Follin et al. 2007 and Follin 2008/. These modelling studies demonstrate that the sheet joints reduce the effects of local topographic variations resulting in flow cells whose scale is more controlled by the extent and inter-connection of structural features, i.e. sheet joints and deformation zones, than topography.

The near-surface groundwater flow in the Quaternary deposits and geosphere-biosphere interface zone has been studied in more detail for a subarea in northern Uppland /Holmén and Forsman 2005/. The study showed that, even though discharge occurs over large parts of the model's top surface, discharge points for particles released at repository depth are confined to a few well-defined low-points in the topography such as below lakes and the sea. Thus, seasonal variations in precipitation (and recharge) greatly govern groundwater flow in the Quaternary deposits, but not the discharge pattern of groundwater flow from larger depths. The near-surface groundwater flow in the Quaternary deposits and geosphere-biosphere interface zone has also been studied in more detail within the SDM-Site project /Bosson et al. 2008/.

3.1.5 Natural analogues/observations in nature

Geochemical, hydrochemical, palaeogeological and palaeohydrological studies can provide insights into long-term and large-scale groundwater flow patterns (see e.g. /Wallin 1995/). Inferences about flow patterns can be made from the distributions of groundwater composition, taking into account the understanding of the overall evolution of the region. Inferences can also be made from the distributions of fracture infill material. If the geochemical information is consistent with the understanding of the flow system, this builds confidence.

Palaeohydrological simulations have become an important tool /SKB 2004b, c, 2005a, b, 2006a, 2008, 2009a/. In these simulations, the evolution of the groundwater flow system and groundwater composition to current conditions is modelled over a suitable time period (such as the period since the last glaciation). The starting conditions for the simulations are plausible conditions based on an understanding of the evolution of the system. If it is possible to develop a consistent picture of the system in this way, then this builds confidence in the models. Indications so far are that the models can be better constrained if several groundwater constituents, including both non-decaying tracers and radioactive tracers (such as tritium) are modelled and used to test the models, rather than just salinity. This is because tracers with different half-lives effectively provide information about the flow at different travel times from the sources of the tracers. For example, tritium enters the groundwater system in recharge, has a half life of about twelve years and mainly originates from the bomb tests in the fifties. Tritium can therefore indicate where groundwater from recharge has moved to in the last fifty years.

3.1.6 Time perspective

The groundwater flow system fluctuates on very short timescales as a result of, for example, tidal effects, rainfall events, seasonal variations in rainfall, and seasonal ground freezing and snowpack development. However, these short-term fluctuations are not relevant to the performance of a deep repository, which is only affected by the average flow system over periods of years or longer. Therefore, the discussion hereafter only addresses this latter issue.

Prior to the investigation of a potential repository site and construction of a repository, the (average) groundwater flow system, although not in equilibrium, will only be evolving very slowly, in response to climate and other environmental changes since the end of the last glacial period. The water table at the sites that have been investigated is currently close to the surface and the salinity at depth is approximately horizontally stratified /SKB 2008a, 2009a/.

The basic pattern of groundwater flow described above will be modified by a deep repository. During construction and operation, a repository will be at atmospheric pressure. Hence, the pressure or hydraulic head at the repository will be much lower than it would have been prior to site investigation and repository construction. As a result, groundwater will be drawn towards the repository and the water table above the repository will be lowered. The water-table drawdown will depend on how permeable the near-surface rocks are relative to the deeper rocks and whether the repository tunnels are intersected by transmissive features that connect to the surface. The drawdown in such features will be reduced if they are grouted.

Groundwater will also be drawn up towards the repository from beneath it. This will lead to upconing of saline water (which could affect the chemical environment around the repository). The upconing in transmissive features that intersect the repository will be less if such features are grouted. Where the repository is very close to the coast (the case at Forsmark initially, less so at Laxemar), saline waters beneath the sea may also be drawn laterally towards the repository. The water that flows into the repository will be removed by a drainage system during repository operation, and hence the perturbed flow pattern outlined above will be maintained.

After the repository has been backfilled and closed, groundwater will continue to flow into the repository for some time. It will start to fill up any void space within the repository, such as the pore space within the backfill, i.e. the repository will resaturate. As the void space fills, the pressure within the repository will rise and the groundwater flow towards the repository will reduce. The water table draw-down above the repository and the extent of saline upconing beneath the repository will both decrease. Ultimately groundwater conditions similar to those before repository construction may be re-established. The time taken would depend on the properties of the rocks. It would probably take tens of years for the water table to return to a level similar to the original (see e.g. /Jaquet and Siegel 2004/). The distribution of salinity might be slightly perturbed by the site investigation, and more significantly perturbed by repository excavation, construction and operation (see e.g. /Hartley et al. 2007/ for the effects of the Äspö HRL on salinity, and /Svensson and Follin 2010a/ for the effects of a repository at Forsmark). It would probably take a period longer than the operation phase for the distribution of salinity to return to one similar to the original.

A repository will also be a source of heat due to radioactive decay of the spent fuel in the canisters. The heat source will largely decay over several hundred years. The heat will lead to buoyancy forces that will modify the groundwater flow in the vicinity of the repository. These buoyancy forces will tend to create convection cells with flow up through the repository and down at some distance from the repository. This flow will be combined with the flow that would otherwise occur.

The thermal buoyancy-driven flow will also tend to increase the extent of saline upconing beneath the repository, and it will act to maintain the saline upconing for longer than would otherwise be the case.

As a result of repository construction and operation, gas may enter the rock pores and fractures immediately adjacent to the tunnel walls. This may be particularly likely if the repository is constructed by ‘drill and blast’ due to the high blast pressures driving gas into rock fissures.

During the assessment period of one million years, the flow system will change as a result of altered climate-related conditions. Climate changes continuously and the climate conditions in Sweden can be expected to change between temperate-, periglacial- and glacial climate domains during the assessment period /SKB 2010c/. The inferred perturbation of natural climate change by the emission of greenhouse gases may, together with known future orbital parameters, result in an extremely long initial temperate period in Fennoscandia and elsewhere. However, over the full assessment period, phases of periglacial- and glacial climate domains will occur at the Forsmark site also in a Greenhouse warming scenario, following a slow return to lower atmospheric greenhouse gas concentrations.

Over such long time periods, the Quaternary deposits might change as a result of reworking beneath an ice-sheet.

The positions of discharge locations would change over time. This would be mainly as a result of the combined effects of the changing surface elevation and changing sea level, leading to changes to the shoreline and the development and/or loss of lakes and rivers. Changes to the Quaternary deposits might also affect the positions of discharge locations.

3.1.7 Handling in the safety assessment SR-Site

The strategy for modelling groundwater flow in the main scenario of SR-Site is outlined below. A combination of CPM/ECPM models and DFN models is used. The CPM/ECPM models represent variable-density flow due to variations in salinity. For fractured rocks represented by an ECPM model, the models represent diffusion of salinity between the groundwater flowing in the fractures and immobile groundwater in the rock matrix between the fractures, and the impact of the resulting changes in density on the flow in the fractures.

The repository tunnels are explicitly included in the models for the excavation/operation and temperate periods, while the tunnels are not included for the periglacial and glacial climate domains. Furthermore, the effect of unsealed investigation boreholes or new boreholes drilled into the repository is analysed.

The application for a final repository for spent nuclear fuel at Forsmark, requires an assessment of the repository design and long-term radiological safety premises. In order to support the evaluation of groundwater pathway over the entire lifetime of the repository, information from a series of three groundwater flow modelling studies that handle different periods is assessed.

- Groundwater flow modelling of the excavation and operation phases – Forsmark /Svensson and Follin 2010a/.
- Groundwater flow modelling of periods with temperate climate conditions – Forsmark /Joyce et al. 2010a/.
- Groundwater flow modelling of periods with periglacial and glacial climate conditions – Forsmark /Vidstrand et al. 2010a/.

The groundwater flow modelling study by /Joyce et al. 2010a/ incorporates an assessment of the impact of unsealed boreholes. In a study by /Bockgård 2010/, the impact of unsealed repository tunnels and shafts is assessed.

A similar series of flow modelling studies is evaluated for Laxemar to support the site selection:

- Groundwater flow modelling of the excavation and operation phases – Laxemar /Svensson and Follin 2010b/.
- Groundwater flow modelling of periods with temperate climate conditions – Laxemar /Joyce et al. 2010b/.
- Groundwater flow modelling of periods with periglacial and glacial climate conditions – Laxemar /Vidstrand et al. 2010b/.

The groundwater situation within each period is modelled separately. That is, the initial conditions for one period are not taken directly from modelling of the relevant previous period. For example, the initial conditions for the start of the temperate climate period are not taken from end of the glacial climate period. The difficulties in representing all climate periods using a single model arise from the need to consider different ranges of processes and length scales during each period. Improving the temporal continuity of the hydrogeological modelling is an objective for ongoing research.

Excavation/operation/resaturation period

This period includes the excavation and operation of the repository and the period after repository backfilling and closure when the repository resaturates. During the excavation and operation periods, the repository tunnels will be at atmospheric pressure, groundwater will flow into the tunnels and the water table will be drawn down towards the repository. After backfilling and closure, water will continue to flow into the repository, the void space within the repository will start to fill up, the pressure within the repository will consequently rise, and the water table will start to return to a level close to its original one before work on the site commenced.

In principle, in order to accurately model the groundwater flow near an open repository, it might be necessary to use a two-phase (air-water) flow model. However, a study carried out by /Painter and Sun 2005/ showed that, although there is a region of two-phase flow in the vicinity of the tunnels before closure, this does not significantly affect the far-field flow or the inflows to the tunnels, which can therefore be evaluated using a saturated groundwater flow model (with the water table represented as a free surface).

The simulations of the excavation, operation and resaturation period are carried out using the computer code DarcyTools /Svensson and Follin 2010a, b, Svensson et al. 2010/. The calculations use a saturated groundwater flow model, with the water table represented by a free surface. Above the water table, DarcyTools prevents horizontal flow above the surface where pressure is atmospheric by reducing the horizontal permeability above this surface. The position of the free surface and the effective hydraulic conductivity are calculated iteratively. Also, DarcyTools employs a simplified treatment of the two-phase flow problem in the resaturation calculations.

The main results of this study are calculations of inflow rates, drawdown of the groundwater table and upconing of deep saline water for different levels of grouting efficiency during the excavation and operational periods of a final repository at Forsmark. Estimates of how long unsaturated conditions might persist within tunnels following the phased backfilling of the repository are also made.

Additional simulations of near-surface effects are carried out using the hydrogeological modelling tool MIKE SHE /Mårtensson and Gustafsson 2010/ in order to asses the interaction between the near-surface and deep hydrogeological systems.

The main inputs to the simulations are the site-descriptive models /SKB 2008a, 2009a/ and the tunnel layouts /SKB 2009b, c/.

Thermal effects (the geothermal gradient in particular) are not addressed in the main simulations for this period, because they have only a minor effect on the drawdown and groundwater inflow to the repository. Scoping calculations of thermal effects have previously been carried out for SR-Can /Hartley et al. 2006a/.

Temperate climate domain

Simulations are carried out for a period of approximately ten thousand years after repository closure and resaturation, up to the expected onset of the next cold climate period using the computer code ConnectFlow /Joyce et al. 2010a, b/. The calculations use a combination of DFN, ECPM and CPM models on a range of scales. Regional-scale ECPM and/or CPM models are used. Major transmissive features (conductive deformation zones) in the region and the backfilled tunnels are represented explicitly. In particular, for the models of Forsmark, the shallow bedrock aquifer resulting from large horizontal fractures/sheet joints in the uppermost part of the bedrock is represented.

The permeabilities of blocks of fractured rock within the CPM model are based on the results of upscaling calculations with DFN models, or simple estimates from measurements. The model takes account of the change in the position of the shoreline over time. The calculations represent the migration of several different water types (effectively several different groundwater constituents) and account for the effect of resulting variations in density on the flow. For fractured rocks, diffusion of the different water types between the flowing groundwater and immobile groundwater in the rock matrix between fractures is represented in the CPM and ECPM models.

A refined region in the vicinity of the repository (repository scale) is modelled as a pure DFN or CPM with boundary conditions derived from the results of calculations with the regional models. In addition, 'canister-scale' DFN and CPM models of a small region in the immediate vicinity of the repository are used and are embedded within the repository scale models. Thus, an explicit CPM representation of the repository tunnels and the deposition holes is embedded in the repository scale models.

In addition, the regional model is used to carry out palaeohydrogeological simulations of the evolution of the groundwater flow system and groundwater chemistry over approximately the last ten thousand years. The effects of the changing shoreline and changing seawater salinity are addressed in these calculations. The results of the calculations are compared with observations to test the model, and the results are used to provide the initial conditions for the calculations for the temperate period. Effectively, this neglects the disturbance to the groundwater flow system during the periods of site investigation, and repository excavation, operation and resaturation.

The main inputs to the calculations are the site-descriptive models /SKB 2008a, 2009a/, and the tunnel layouts /SKB 2009b, c/.

Although the main calculations for this period account for the effects of the background geothermal gradient on groundwater density and viscosity, they do not address the effects of buoyancy-driven flow resulting from the heat generated by the radioactive waste within the repository. This is because the effects were found to be small in scoping calculations that quantified this effect in SR-Can /Hartley et al. 2006a, b/.

Further, the main calculations for this period do not address the impact of gas flow. This is because its impact is expected to be small, because the rate of gas generation is small. Scoping calculations of the effect of bubble gas flow on the groundwater flow were carried out to address this issue for SR-Can /Hartley et al. 2006a, b/.

In the main calculations, the unsaturated region near the ground surface was not modelled because it has a minor effect on the flows in the deep rocks. However, the unsaturated zone was taken into account in calculations of the near-surface hydrology carried out using MIKE SHE /Bosson et al. 2008, Mårtensson and Gustafsson 2010/. These calculations were used to determine the maximum potential recharge (precipitation less evapotranspiration), which was a control on the boundary condition on the upper surface of the ConnectFlow models.

Periglacial climate domain

In the SR-Site assessment, calculations are carried out to assess the groundwater flow pattern during a period when there is permafrost in the near-surface rocks, which will act as a barrier to groundwater flow. The DarcyTools code is used for these simulations /Vidstrand et al. 2010a, b/. The main input to the simulations is the site-descriptive models /SKB 2008a, 2009a/. The evolution of permafrost is modelled using DarcyTools, and the results are compared to more elaborate (two-dimensional) simulations of permafrost carried out as part of the study of climate evolution /Hartikainen et al. 2010, SKB 2010c/.

Calculations are also carried out to examine the movement of saltwater arising from salt exclusion during freezing beneath an advancing permafrost front /Hartikainen et al. 2010/.

Glacial climate domain

Calculations are carried out to examine the groundwater flow and flow paths in the environment of a repository in fractured rock during the advance and retreat of an ice sheet. (The effects of periglacial permafrost, the case described above, are considered in a variant). The calculations are undertaken with the DarcyTools code /Vidstrand et al. 2010a, b/. The main inputs to the calculations are the site-descriptive models /SKB 2008a, 2009a/, and the configuration of the ice sheet, which comes from theoretical/empirical conservative estimates of ice thicknesses. Additional information about the ice sheet is obtained from an ice-sheet model, see /Näslund et al. 2010/ and the SR-Site Climate report /SKB 2010c/.

The calculations are carried out with a model covering an even larger domain than the regional model used in the SDM-Site project. The ice sheet is taken to impose a pressure boundary condition on the top surface of the model. This boundary condition results in the occurrence of both recharge and discharge beneath the ice sheet. In heterogeneous bedrock, highly transmissive fracture zones could act as conduits for flow, feeding groundwater up or down beneath the ice sheet (see for example /Vidstrand et al. 2010a, Section 7/). Cases with ice sheets overlying permafrost or in direct hydraulic contact with groundwater are considered. The modelling assesses a series of groundwater flow situations for several different ice front locations relative to the repository location at different stages of the ice sheet advance and retreat. A sensitivity study investigates the impact of different ice sheet flow directions, different hydraulic properties, different ice sheet thicknesses, and different temperatures at the ice-subsurface interface close to the ice sheet margin.

Earthquakes

The effects of earthquakes on groundwater flow have not been considered in SR-Site. However, simplified calculations of radionuclide transport have been performed (see Section 6.1.7).

3.1.8 Uncertainties

An assessment of the confidence that can be placed in the current site descriptive models of Forsmark and the remaining uncertainties is described in /SKB 2008b/, and there is a corresponding document for Laxemar /SKB 2009f/. A large number of boreholes have been the subject of core, image and hydraulic test logging using the Posiva Flow Log (PFL) method to give high spatial resolution in the characterisation of flow conducting features. These show a consistent picture and confirm the existence and extent of the low permeability volumes at depths in the key fracture domains of interest. On this basis, there is generally high confidence in the overall hydrogeological conceptual model, which has been further supported by a number of confirmatory tests considering interference tests, predictions of newly drilled boreholes and modelling of palaeohydrogeology to compare simulations of the evolution of groundwater composition over the current Holocene temperate period with hydrochemistry data (see /Follin 2008, Follin et al. 2008/. The essential hydraulic properties of relevant bedrock volumes are captured by the PFL-testing, both in terms of bulk flow capacity and variability of local flow within the connected fracture network. The DFN models developed in the SDM reflect these flow characteristics and are calibrated against statistics measuring the bulk flow and local flow variability.

There are, however, various uncertainties remaining in the hydrogeological site description and in evaluating the groundwater flow system over the periods that need to be considered in the assessment.

Uncertainties in mechanistic understanding

The process of groundwater flow is well understood and the models for groundwater flow are generally well accepted. The underlying model for groundwater flow takes this to be predominantly through channels in fractures. Perhaps the main uncertainties about models for groundwater flow are about the appropriate models for two-phase flow and unsaturated flow in fractured rocks. The models outlined in Section 3.1.1 are those generally accepted. There is a good understanding of heat transport and the model outlined in Section 3.1.1 is the standard model for this process.

There is an adequate conceptual understanding of the way in which mechanical and chemical processes (such as the loading of an ice sheet and mineral precipitation or dissolution) influence groundwater flow through modifications to the rock properties, but there is considerable uncertainty about the way in which to model these effects quantitatively. However, these processes are expected to have little effect during the temperate period.

There are considerable uncertainties in the description of basal processes in ice-sheet models, see the SR-Site Climate report /SKB 2010c/. These lead to uncertainties about the conditions at the base of an ice sheet, such as the magnitude and extent of recharge to the groundwater flow. These uncertainties then lead to uncertainties about the groundwater flow in glacial periods.

Parameter uncertainties

There are remaining uncertainties in the spatial variation of hydraulic properties of the rock mass in the potential repository volume. The spatial variability of hydraulic properties affects the distribution of flow and consequent transport processes in groundwater. At Forsmark the majority of flow-conducting fractures detected by the PFL method are associated with deterministic deformation zones, while at Laxemar there are many flow-conducting fractures outside of deformation zones. A Poisson point process for the spatial distribution of flow-conducting fractures is assumed in the hydrogeological DFN models, although in reality there may be structure to the variability in fracture occurrence. Some such structure is captured by dividing the rock mass into fracture domains and depth intervals, but structured variability within each subdivision may still exist. The variability in local flow is measured by the extensive PFL testing, and statistics of these variations are reproduced in the DFN models. However, the spatial structure of the variations, such as any correlation between fracture size and transmissivity, cannot be determined. Such uncertainties are addressed by considering a range of alternative statistical models. For a particular statistical model, there will be uncertainty about its parameters, even when a model is calibrated against available measurements, because the number of measurements that can be made is finite. The distribution of flow within an individual fracture and the size distribution of fractures within a network cannot be determined directly from surface investigations. Such issues can again be addressed by considering alternative models, using the available PFL test and interference test data to constrain the connectivity characteristics of each model.

Although much effort has been focussed on characterising the positions and properties of deformation zones in the site investigations, measurements suggest large spatial variability in their properties, and hence uncertainty in their properties away from the boreholes. Their properties have some importance during the open repository period since they affect the extent of grouting needed and also affect drawdown and saturation. However, their contribution to retention in the geosphere is considered to be limited since the flow-related transport resistance in large deformation zones is assumed to be relatively low. However, uncertainties in the hydraulics of the deformation zones have more significance for the evolution of groundwater composition and the locations of discharge to the biosphere.

Hydraulic properties of the rock mass and deformation zones outside the area of focus for borehole drilling are much more uncertain, although the significance of such volumes and structures in respect of groundwater composition and radionuclide transport is expected to be reduced. Potentially they have greater relative importance during periods of ice sheet advance and retreat when the size of flow cells is likely to increase due to the dominance of the regional hydraulic gradient associated with the front of the ice sheet.

There is some uncertainty about the detailed variation of the hydrogeological properties within the Quaternary deposits, and about long-term changes to these.

Another source of uncertainty lies in the constitutive relations (the relation between relative permeability and saturation and the relation between pore pressure and saturation) used in CPM representations of unsaturated flow and two-phase flow in fractured rock. The characteristic curves cannot be directly measured for a fractured rock.

Model simplification uncertainties in SR-Site

In the modelling carried out for SR-Site, various simplifications are made.

The unsaturated zone is not represented in the modelling of the temperate and glacial climate periods, although a free surface algorithm is used to model the elevation of the ground water table in the calculations for the excavation, operation and resaturation period /Svensson and Follin 2010a/. The algorithm reduces the horizontal flow above the groundwater table. In general, neglecting the unsaturated zone is considered to be a minor approximation within SR-Site, because the groundwater table is expected to be close to the ground surface for most of the period after repository resaturation.

The region of two-phase flow in the immediate vicinity of the repository prior to resaturation is not modelled explicitly. However, the study by /Painter and Sun 2005/ showed that a saturated flow model with the water table represented as a free surface gave good results for the far-field flow and the inflows to the tunnels in this case. The calculations of the excavation and construction period for SR-Site /Svensson and Follin 2010a/ implement a free surface approach in their estimates of tunnel inflows and groundwater drawdown.

Thermal effects are neglected in the calculations for the excavation, operation and resaturation period. This is considered to be a reasonable approximation because the effects of the temperature distribution on the drawdown and groundwater inflow to the repository, which are the key issues for this period, are relatively small. The effects of buoyancy-driven flow generated by the heat from the waste are not taken into account in the main calculations for the period after closure and repository resaturation. However, scoping calculations of the effects of the thermal buoyancy-driven flow are undertaken. This is considered an appropriate level of treatment, since there are not expected to be significant releases of radionuclides during the period when thermal effects are greatest.

Diffusion of salinity into or out from the rock matrix is taken to be at constant density. This is judged to be a minor approximation, because the variations in salinity are fairly small and correspond to variations in the effective diffusion coefficient in the rock matrix that are small, and considerably smaller than the uncertainty about the effective diffusion coefficient.

The model adopted for the transport of groundwater constituents during the temperate period treats all constituents as conservative (not interacting with the rock) and non-decaying and takes the dispersion for a particular constituent to be proportional to its concentration gradient. These approximations allow the transport to be modelled as transport of fractions of reference waters. The first approximation is judged to capture the main aspects of the transport, and indeed some of the key groundwater constituents, such as chloride and oxygen isotopes are, in fact, conservative. The second approximation is judged to be minor.

In the DFN modelling, fractures are taken as planar rectangular features. A fracture is either taken to have a constant transmissivity, or the variation in transmissivity over a fracture is taken to be based on a simple rectangular subdivision of the fracture with constant transmissivity in each subdivision. As noted, the flow is considered to be through channels in fractures. The flow modelling with DarcyTools and ConnectFlow may not give a detailed representation of the channels. This might be better achieved by channel models, although there may be difficulties in estimating the parameters for such models. However, it is judged that the ConnectFlow and DarcyTools models capture the main characteristics of the fracture flow system, such as flow occurring through an often sparse network of discrete fractures of varying size and transmissivity.

Boundary conditions are approximated in various ways. For example, the lateral boundaries of the regional model are taken to correspond to groundwater divides for all time. The boundary condition for salinity on the top surface of the model onshore is taken to be zero salinity. These are judged to be minor approximations.

There are also uncertainties resulting from the use of numerical models for the groundwater flow calculations. These are judged to be minor given the levels of refinement in the models.

Input data and data uncertainties in SR-Site

There are uncertainties about the evolution of the distribution of salinity. However, calculations of the future evolution of the repository system are based on the current distribution. In turn, this is based on a combination of extrapolation from current observations and calculations of the evolution of the current distribution from a plausible assumed distribution immediately after the last glaciation. The calculated distribution is tested against current observations to build confidence in it.

There are uncertainties about conditions beneath ice sheets, although considerable strides in understanding have been made in recent years through modelling and experimental studies, see Climate report /SKB 2010c/.

There are uncertainties about future climate-related conditions, particularly taking into account the possible impact of increased global warming.

3.1.9 Adequacy of references supporting the handling in SR-Site

The code ConnectFlow /Hartley and Holton 2004/ is developed within a QA programme approved under ISO 9001: 2000 and the reference is a report that was developed within the framework of a QA system that requires a documented factual and quality review before approval and printing, and has undergone such a review.

The reference /Jackson et al. 2000/ supporting the use of CPM models to represent, on suitable length scales, groundwater flow in rocks through which groundwater flows predominantly through fractures, is a peer-reviewed article that is available in the open literature (in a journal that is widely regarded as the premier journal for publishing work on hydrogeology). It is based on work that was carried out within a QA programme approved under ISO 9001: 2000. The other references /La Pointe et al. 1995, Svensson and Ferry 2004/ supporting this approach are SKB reports. They are scientifically consistent with the report /Jackson et al. 2000/ and are therefore considered to provide additional support for the approach.

The references /Hartley et al. 2005a, b/ supporting modelling of several groundwater constituents are reports that were developed within the framework of a QA system that requires a documented factual and quality review before approval and printing, and they have undergone such review. The reference /Rhén and Smellie 2003/ supporting modelling of several groundwater constituents is the final report from an international project, and was subject to peer review by the participants within the project. It is scientifically consistent with the references /Hartley et al. 2005a, b/ and therefore is considered to provide additional support for these references.

The reference /Laaksoharju et al. 2008b/, describing the use of the reference water concept, is an SKB report that has undergone documented factual and quality review.

The most recent reference for the DarcyTools code /Svensson et al. 2010/ is based on /Svensson 2004/. The latter report is an SKB report that has undergone documented factual and quality review and discusses how a CPM model can give a good representation of a rock in which groundwater flow predominantly through fractures.

The reports /SKB 2010c/ describing climate related issues, and /SKB 2010f/ describing the impact of human activities on the groundwater flow are SKB reports prepared for SR-Site that have undergone documented factual and quality review.

The references /SKB 2008a, 2009a/, which report the site-descriptive models of the sites Forsmark and Laxemar, respectively, including descriptions of the current position of the water table and the variation of the salinity with depth, are SKB reports that have undergone documented factual and quality review.

The reference /Jaquet and Siegel 2004/, which discusses the time for the water table to return to conditions similar to those before repository construction is an SKB report that has undergone documented factual and quality review, although not according to the procedure defined for SR-Site reports.

The reference /Painter and Sun 2005/, which discusses the modelling of an open repository, is an SKB report that has undergone documented factual and quality review. However, the SR-Site procedures for review, including formal review protocols, have not been followed; instead, a more free format review was undertaken.

The references /Svensson et al. 2004, Svensson and Ferry 2004, Svensson 2004/ which discuss the Darcy tools code are SKB reports that have undergone documented factual and quality review.

The references /SKB 2009b, c/ describing tunnel layouts are SKB reports that have undergone documented factual and quality review.

The reference /Hoch and Jackson 2004/ describes how matrix diffusion is implemented in the ConnectFlow software. This work was carried out within a QA programme approved under ISO 9001: 2000 and the reference is a report that was developed within the framework of a QA system that requires a documented factual and quality review before approval and printing, and has undergone such a review.

3.2 Gas flow/dissolution

3.2.1 Overview/general description

This subsection is concerned with the migration of species present in the geosphere that are generally considered to be gases; that is, species that would, if on their own, exist as free gases under the ranges of temperature and pressure found in the region of the geosphere of interest. Typical such gases include nitrogen, oxygen, hydrogen, methane, carbon dioxide, and the noble gases. In the geosphere, these gases may be present in a gaseous phase or dissolved in groundwater (or potentially sorbed on to rock, although this is neglected as of no significance for gases).

It should be noted that the presence of a gas phase can cause some gases (not initially present in the gas phase) that would otherwise remain dissolved in the groundwater at the prevailing pressure to partially partition into the gas phase. This “stripping” of gases from solution is discussed in Section 5.10.1. The quantities of radioactive gases that are present are expected to be far too small for them to form a gas phase on their own; other gaseous compounds are needed to create the gas phase.

A gas phase can form if the sum of the partial pressures of all constituent substances in the water exceeds the prevailing pressure (plus any capillary pressure). The composition of the gas phase will be such that the partial pressures of the component gases are in equilibrium with their modified groundwater concentrations. The natural concentrations of dissolved gases, for example nitrogen and helium /Hallbeck and Pedersen 2008b/, are, however, so low that they are not typically sufficient to form a gas phase at the water pressure prevailing at the depths in question, as shown in Table 3-2.

Higher gas concentrations could arise in the vicinity of a defective canister if water ingress through the defect leads to corrosion of the iron insert. Hydrogen gas is generated by oxygen-free corrosion of iron, and it is likely that the generation of this gas would cause the water local to the deposition hole to become saturated with dissolved gas and for bubbles of free gas then to be formed. Since gas bubbles are less dense than water, they will tend to move upward towards the biosphere. The bubbles may coalesce to form a more continuous gas phase, but the principle of mainly vertical gas migration under the influence of buoyancy will still apply.

The possibility that migrating gas may modify groundwater flow velocities in the neighbourhood of the migrating gas and thereby influence transport of radionuclides dissolved in groundwater is discussed in Section 6.1.

Table 3-2. Measured dissolved natural gas concentrations at Forsmark /Hallbeck and Pedersen 2008b/ and estimated solubilities at 400 m depth.

Gas	Measured concentration (mol/m^3)	Approximate solubility at a depth of 400 m (mol/m^3)
Nitrogen	< 6	31
Helium	< 2	15
Methane	< 0.2	72
Carbon dioxide	< 0.2	1,900
Hydrogen	< 0.02	33

Sources of gas

Three possible sources of the gases present in the geosphere are considered: natural gases, gases generated from materials deposited in the repository; and air that, during repository operations, is present in repository structures and is introduced into the surrounding rock and is then trapped there at repository closure.

Groundwater generally contains varying quantities of naturally dissolved gas /Pedersen 2001/. In Swedish groundwaters, nitrogen is usually the dominant gas present, followed by methane, carbon dioxide, helium, argon, and hydrogen. Sometimes, high concentrations of hydrogen and methane occur. The total quantity of dissolved gas varies around 5 volume-percent (NTP[3]) and is generally higher towards greater depth. There are sites where very high gas concentrations have been encountered, up to 1 litre of gas per litre of groundwater, and where the gas composition is completely different, with hydrogen and/or methane as the dominant components /Sherwood et al. 1993, Pitkänen et al. 2004/.

At the Forsmark and Laxemar sites, nitrogen followed by helium are present in the greatest amounts, with nitrogen and carbon dioxide being most common in the more shallow groundwaters and helium in the deeper parts of the system /SKB 2008a, 2009a/. This and the origin of natural gases in the geosphere are further discussed in Section 5.10.

Repository processes that are expected to generate gases include radiolysis of water and metal corrosion. Both these processes produce hydrogen. In a Swedish repository for spent fuel, the generation of hydrogen by anoxic corrosion of iron in a spent fuel canister can occur only in the unlikely event that the copper canister is breached, and then is expected to be the main source of gas. The generation of gas within the repository is discussed in the following process-description reports: spent fuel processes for radiolysis of water and canister processes for iron corrosion /SKB 2010d/, and buffer processes and backfill processes for rock bolt corrosion /SKB 2010e/.

During the excavation and operation phases of the repository, it may be expected that parts of the excavation damaged zone (EDZ) and rock near the tunnels will dry out and become unsaturated. This might occur, even though there is a large prevailing hydraulic pressure gradient driving groundwater towards the open repository, if the rock is poorly fractured and the rock matrix has very low hydraulic conductivity. The air in the EDZ and neighbouring rock will be entrapped at repository closure. However, this amount of air added to the repository system is negligible when compared with the volume of air trapped in the unsaturated porosities of the buffer and the backfill. Free gas that is trapped in the repository at repository closure will be at atmospheric pressure. This means that the volume of gas will be drastically reduced when the repository resaturates and the pressure is restored to the hydrostatic value at the repository depth. An increasing quantity of this gas will also dissolve in the groundwater as the pressure rises on resaturation (see below).

Earlier generic calculations by /Painter and Sun 2005/ suggested that, during repository operations, water flow into the repository would cause the water table above the repository to drop to the level of the repository[4]. The consequence would be a larger volume of gas in the host rock than that simply from desaturation of the rock close to the repository itself. The modelling of the excavation and operation phases at Forsmark performed for SR-Site /Svensson and Follin 2010a/ applies the site specific bedrock conditions interpreted in SDM-Site Forsmark estimates maximum drawdowns around 10 metres depending on grouting efficiency. The differences for these estimates are believed to result from the much higher permeabilities (two orders of magnitude higher) of the deep bedrock used in /Painter and Sun 2005/ and their neglect of the grout that would be applied in the tunnels shortly after excavation. Hence, desaturation is expected to take place predominantly in the immediate vicinity of the repository.

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[3] NTP, or normal temperature and pressure, is taken here to denote conditions of 25°C and 1 atmosphere pressure, particularly for measuring gas volumes. Alternative conditions, STP, or standard temperature and pressure, are sometimes invoked, in which the temperature is taken to be 0°C. This distinction is not material to the discussion presented here.

[4] However, such behaviour has not been observed at, for example, the Äspö HRL.

Physical state of gaseous compounds

As already indicated, gases may be present in the geosphere as a free gas phase or in solution in the groundwater (both in the fractures and in the rock matrix). A discussion of the factors controlling the partitioning of gases between solution in groundwater and existence as a free gas phase is provided in Section 5.10. It suffices for the purposes of this section to note that, to a good approximation, the solubility of a gas is proportional to the gas pressure (Henry's Law), so that some of the gas that was in solution at the pressure pertaining at the repository depth might come out of solution if the water containing the gas moved to a lower pressure region.

Equally, gas that is initially present as a free gas phase, because the water with which it is in contact has become saturated with dissolved gas, may subsequently dissolve if it migrates to a region in which the groundwater is not saturated with the gas or gases in question, or if the saturated groundwater is replaced by fresh groundwater as a result of groundwater flow.

Consequences of appearance of free gas

Chemically non-reactive gases that remain in solution in groundwater are not considered to have any particular consequences for repository performance that are peculiar to the fact that they can exist as a gas phase. The appearance of a free gas phase, that may either be trapped local to the repository or migrate through the geosphere away from the repository, may introduce new effects, leading to the identification of a number of potential consequences for repository performance /Rodwell et al. 2003/, as discussed in the following paragraphs.

Gas generation in the repository may cause a build up of gas pressure in the repository and host rock. If the pressure were to rise sufficiently, damage to engineered structures or fracturing of the host rock might occur. The potential for such overpressurisation to occur depends on the gas generation rate and the gas transport capacity of the near field materials and the host rock. For a Swedish spent fuel repository, the barrier likely to provide the main impediment to gas release from the repository is the bentonite buffer, which is discussed elsewhere /SKB 2010e/.

A migrating free gas phase may include radioactive, toxic, or flammable gases, and transport of these to the surface in the gas flow may lead to human exposure to radiation, toxic materials or to flammability hazards. The transport of volatile radioactive compounds in a free gas phase is discussed in Section 6.2. For the spent fuel repository, the rate of generation of hydrogen, the only flammable gas likely to be produced, is too small to present a flammability hazard at the surface, and no toxic gases that might pose hazards at the surface have been identified as potentially arising from the wastes.

The presence and migration of a free gas in the geosphere may modify groundwater flows and hence the transport of dissolved radionuclides. Most obviously, the presence of a body of trapped gas could provide a barrier to groundwater flow; this might be particularly the case close to the repository. Several studies have suggested that flows of gas through fracture networks might induce groundwater flows. Two mechanisms have been suggested by which this might occur; by the collapsing and reforming of gas pathways, and by the entrainment of groundwater in streams of bubbles. Also, in principle, the presence of gas bubbles, which reduces the effective density of the water, leads to buoyancy forces, which can drive groundwater flow. Further discussion of these mechanisms and references can be found in /Rodwell et al. 1999/. However, no clear demonstrations of these effects in the field, or their quantification, are available. It is not thought likely that the quantity of gas produced in a Swedish spent fuel repository would be sufficient for these effects to be significant.

Gas migration in the form of bubbles may also affect radionuclide transport by the attachment of material to bubble surfaces. This is discussed in Section 6.2.

Finally, gases may take part in chemical reactions in the geosphere, but any significance such reactions might have is dependent on the chemistry of the gases rather than the fact that they are gases. Reactions of gases in the geosphere are discussed in Section 5.10.

Gas flow/transport of dissolved gas

Free gas generated in defective spent fuel canisters will, when its pressure has risen sufficiently high, first have to migrate through the bentonite buffer around the canisters. There are various paths it could then follow. If there are conducting fractures intersecting the deposition hole, gas could enter the geosphere fracture network directly through these fractures. Alternatively, the gas could pass vertically into the deposition tunnel, where it could move laterally along the tunnel or the EDZ around the tunnel until encountering rock fractures which it could enter. The EDZ may have a higher conductivity than the rock and so provide a preferential route for the gas, except that the main driving force for gas flow is expected to be the buoyancy arising from its low density compared with water and this will cause the gas movement to be preferentially upwards, out of the tunnel or EDZ into the rock fractures. Gas could also collect in the tunnel, if there are sections of the tunnel where the roof is not intersected by flowing fractures or the narrowness of the fracture apertures and capillary forces restrict gas entry. Throughout its migration, there is the possibility that some of the migrating gas could dissolve in the local groundwater; the extent to which this occurs will depend on the amount of water that the free gas may interact with and how close this groundwater is to being saturated with gas.

The CPM approach described in Section 3.1 for modelling groundwater flow using Darcy's law is generalised to two phase gas-water flow by modifying the water equation to take account of the interactions between the two phases, as described in the following paragraphs, and introducing a similar equation for the gas phase. A more detailed account of gas-phase flow phenomena in relation to radioactive waste repositories can be found, for example, in the compilations by /Rodwell et al. 1999/ and /Åhlén 2004/, and, in relation to fractured rock, specifically in the summary provided in /RETROCK 2004/.

In a gas-water system, the specific discharge vector, $\mathbf{q}_f$, for phase f is given by:

$$\mathbf{q}_f = -\frac{k k_{rf}(S_g)}{\mu_f}\left(\nabla p_f - \rho_f \mathbf{g}\right) \qquad f = w, g \tag{3-10}$$

where k is the rock permeability, k_{rf}, μ_f, p_f, and ρ_f are respectively the relative permeability, viscosity, pressure, and density of phase f, with $f = w$ and g for water and gas respectively. S_g is the gas saturation and $\mathbf{g}$ is the gravitational acceleration vector.

The phase pressures are related by:

$$p_g - p_w = p_c(S_g) \tag{3-11}$$

These equations involve the relative permeabilities and the capillary pressure (p_c, discussed below), which are functions of the gas saturation, the fraction of the pore volume occupied by gas.

The two-phase flow equations consist of these equations together with the equations of mass conservation for each phase. It should be noted that, for the gas phase, it is necessary to take into account the dependence of the density on the pressure. For an ideal gas, which is a good approximation for the ranges of conditions considered, the density is proportional to the pressure.

As indicated, the capillary pressure relates the pressures in the two phases. On the small scale, capillary pressure represents the pressure difference across the curved meniscus separating gas and water phases. For a fracture containing gas and water, assuming that the water wets the fracture surfaces, as is usually the case because water is typically more strongly bound to rock than gas, the capillary pressure is usually calculated as:

$$p_c = \frac{2\sigma}{a} \tag{3-12}$$

where σ is the surface tension of water and a is the local fracture aperture.

Because of the capillary pressure, the gas pressure has to exceed the water pressure to displace water from pores and fracture spaces, and the smaller the pores or fracture apertures, the greater the pressure difference needs to be for the gas to displace the water. For a given capillary pressure in a rough fracture, the gas will (neglecting gravitational and viscous forces) fill the fracture until the gas-water interface follows the line marking the boundary between accessible areas of the fracture with apertures greater than the value given by the above equation and areas with smaller apertures. On larger scales than pores and fractures, the capillary pressure leads to gas only displacing water from the rock if the pressure in the gas exceeds that in the water by a certain amount: the gas entry pressure.

The effect of capillary pressure is for the gas to first occupy the large pore spaces and to invade increasingly small spaces (i.e. the gas saturation rises) as the gas pressure increases (relative to the water pressure). This is a dynamic situation, with the pressure build up, and hence the degree of gas saturation, depending on the balance between the rate of gas production and the rate of gas migration. The contribution of the capillary pressure to the driving forces for two-phase flow is generally to cause water to flow from "wetter" to "dryer" areas; that is, to oppose the build up of local gas saturation in favour of gas migration to other regions with lower capillary pressures. The static relationship between degree of saturation and pressure for gas and water is strongly dependent on the fracture aperture variability and pore geometry of the rock. Experimental data on the capillary pressure are required for calculations.

The relative permeability for each phase is a modifier to the permeability that takes account of the proportion of the pore space occupied by the phase and the spatial interference between the two flowing phases. As would be expected, the relative permeability is strongly dependent on the degree of saturation for the phase. This is particularly true for water, where the conductivity decreases rapidly with even a small presence of gas in the system. This is due to the fact that the large fractures and pores, which represent the greatest contribution to the conductivity, are rapidly emptied since the water is not so tightly held by capillary forces there. The gas, on the other hand, occupies the large pores, so that it might be expected that the conductivity of the gas would rise rapidly at even a moderate degree of saturation. This is reflected in the relative permeability functions that are assumed by some authors. However, some studies, mainly of a theoretical nature (e.g. /Pruess and Tsang 1990, Persoff and Pruess 1995, Mott and Rodwell 1998, Swift and Goodfield 2001/), have suggested that, in the two-dimensional geometry of a fracture, the interactions between the two flowing phases, gas and water, restrict the relative permeability of each phase, so that the relative permeability for the gas remains zero until a significant gas saturation has been achieved. The two-dimensional nature of rock fractures may entail a greater channelling of the water flow compared with the two-phase conditions in three-dimensional media (e.g. /Jarsjö 1998, National Research Council 1996/). The dependence of the conductivity on the degree of saturation for the phase in question needs to be determined experimentally if quantitative calculations are to be made.

The water pressure in a groundwater system may be written in terms of the hydrostatic pressure and a residual pressure, p'_w,

$$p_w = \rho_w g z + p_{w0} + p'_w \tag{3-13}$$

where z is the depth below datum, p_{w0} is the water pressure (assumed fixed) at the datum level, and it is assumed for presentational purposes that the water density is constant. Using this expression in the above equations gives:

$$\begin{aligned} \mathbf{q}_g &= -\frac{k k_{rg}(S_g)}{\mu_g}\left[\nabla p'_w + \nabla p_c(S_g) + (\rho_w - \rho_g)\mathbf{g}\right] \\ &\approx -\frac{k k_{rg}(S_g)}{\mu_g}\left[\nabla p_c(S_g) + (\rho_w - \rho_g)\mathbf{g}\right] \end{aligned} \tag{3-14}$$

(because the gradients of p'_w are generally small compared to the other terms). This equation shows the contribution that buoyancy forces make to the gas flow. Buoyancy will dominate the direction of gas flow on the large scale, but capillary pressure will determine the distribution of the gas phase within fractures along the flow path. The effect of buoyancy, in particular, means that the direction of free gas-phase flow may not be in the same direction as the groundwater flow. Where there is a constriction in the aperture of a sub-vertical channel in a fracture, gas may spread out below the constriction until the gas pressure has risen sufficiently to force the gas through the constriction. A gas cushion will build up with a thickness such that the hydrostatic head across the cushion is equal to the capillary pressure associated with the constriction. Viscous pressure gradients may be important, as gas pathways through the geosphere are initially created, as gas displaces the water.

Note that the Darcy flux relates to the volume flow of gas at the local pressure. For a given mass flow rate, the corresponding volume flow rate will increase with decreasing pressure because of the compressibility of the gas.

Although the porous medium flow Equations (3-10) to (3-14) are used to describe gas-water flow in fractured rock, there are some difficulties with their application.

First, it is difficult in practice to determine the capillary pressure and relative permeability functions on the scale needed for field-scale numerical modelling for a fracture network.

Secondly, there may be important features of the flow, particularly small-scale features that are not captured by the two-phase flow equations. Gas transport as discrete bubbles that are small compared to the numerical discretisation (which will always be the case for field-scale modelling) is not properly captured by these equations. Gas migration may also exhibit instabilities of various forms: viscous and gravitational instabilities which lead to "fingering" of gas flow and accelerated advance through the fracture network; and instabilities concerned with the creation and collapse of gas flow channels through the fracture network. The latter may be significant as an effect on water movement that is not captured by the large-scale application of the porous medium flow equations.

These issues are discussed in more detail by /Rodwell et al. 1999/ (see also the summary in /RETROCK 2004/).

There is an implied assumption in the two-phase flow equations that when a gas phase is present it is connected, so that the viscous pressure gradient in the gas phase is well defined. Where flowing gas breaks up into bubbles, this is no longer the case.

Although there are some difficulties in the quantitative application of the general two-phase flow equations to a fractured rock geosphere, the understanding that is available of the mechanisms of gas migration should allow simple arguments to be developed to adequately bound the capacity of the geosphere to transport a free gas phase from the repository to the surface. Except possibly in an exceptionally low permeability rock, it is expected that free gas generated from spent fuel wastes will easily be able to disperse through the geosphere. Calculations within SR-Can /Hartley et al. 200a, Section 5.2/ found that a single fracture intersecting each deposition tunnel with an aperture of $15 \cdot 10^{-6}$m (equivalent to a transmissivity c. 10^{-9} m^2/s) was sufficient to carry the estimated upper bound for gas generation from a defective canister to the surface, and concluded such conditions were met by the fracture network at Forsmark.

The two-phase flow around the repository excavations during operations is of a somewhat different nature to that of a gas migrating through an initially saturated fracture network after repository closure. During the operational phase, the gas in the unsaturated zone is connected to the air in the repository at atmospheric pressure, and it is a good approximation to assume that the gas pressure in the unsaturated zone is constant at this value. This leads to simplified equations for water movement and the variation of gas saturation in the unsaturated zone during operations. However, issues connected with the presence of gas in the geosphere are only likely to be of significance after the repository has resaturated.

Gas that is dissolved in the groundwater is transported along with the groundwater in the same way as any other solute. Transport may occur both by advection and by dispersion/diffusion. The only additional issue arising in the case of gas is, as already mentioned, that gas might come out of solution if the water pressure is reduced sufficiently, usually as the water moves towards the surface. This phenomenon will give rise to a two phase flow situation.

3.2.2 Dependencies between process and geosphere variables

Table 3-3 shows how gas flow is influenced by and influences geosphere variables and other processes. The handling in SR-Site is also indicated in the table and further described in Section 3.2.7.

Table 3-3. Direct dependencies between the process "Gas flow/dissolution" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Temperature in bedrock	Yes. Affects gas viscosity.	Excavation/ operation/ resaturation	Air flow down into the region where the water table is drawn down and subsequent flow back is not modelled explicitly but taken into account through models in which the water table is treated as a free surface. No repository generated gas is included. Effect of the gas phase taken into account explicitly in resaturation calculations using a simplified model of gas and water phase flow.	Yes, in principle. But heat transport through gas flow negligible compared with transport by conduction, see Section 2.1.	Excavation/ operation/ resaturation	Neglected because very small and gas flow minor process.
		Temperate	Properties at constant temperature.		Temperate	Neglected because very small and gas flow minor process.
		Periglacial Glacial	Gas flow neglected; minor process.		Periglacial Glacial	Neglected because very small and gas flow minor process.
Groundwater flow	Yes. Groundwater flow and gas flow are coupled and flowing groundwater can transport dissolved gas, which may subsequently come out of solution.	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above) except for resaturation phase. No repository generated gas.	Yes. Groundwater flow and gas flow are coupled.	Excavation/ operation/ resaturation	Minor process, see Section 3.1 Groundwater flow.
		Temperate	Considered in estimates of the capability of the geosphere to transport gas /Hartley et al. 2006a/.		Temperate	Effect of gas bubble flow on the water flow (by entrainment of water) is taken into account in scoping calculations of gas flow /Hartley et al. 2006a/.
		Periglacial Glacial	Neglected; minor process.		Periglacial Glacial	Neglected; minor process.
Groundwater pressure	Yes. See row Groundwater flow above.	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above) except for resaturation phase. No repository generated gas.	Yes. Groundwater flow (which determines the groundwater pressure) and gas flow are coupled.	Excavation/ operation/ resaturation	Gas flow neglected; minor process (see row Groundwater flow above).
		Temperate	See row Groundwater flow above.		Temperate	See row Groundwater flow above.
		Periglacial Glaciation	Neglected; minor process.		Periglacial Glacial	Neglected; minor process.
Gas phase flow						

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Repository geometry	Yes. Affects the distribution of gas flow paths in the geosphere.	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above) except for resaturation phase. No repository generated gas.	No. Does not directly affect the geometry of deposition holes and tunnels.	–	–
		Temperate	Deposition tunnel geometry considered in estimates of the capability of the geosphere to transport gas /Hartley et al. 2006a/.			
		Periglacial Glacial	Neglected; minor process.			
Fracture geometry	Yes. Geometrical configuration of fractures governs the gas flow.	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above). No repository generated gas.	Yes. In principle, gas pressure could induce rock fracturing.	Excavation/ operation/ resaturation	Gas flow neglected; minor process.
		Temperate	Site-specific DFN model in estimates of the capability of the geosphere to transport gas /Hartley et al. 2006a/.		Temperate	Neglected; scoping calculations show that gas can be transported away from the repository without requiring a larger overpressure /Hartley et al. 2006a/.
		Periglacial Glacial	Neglected; minor process.		Periglacial Glacial	Neglected; minor process.
Rock stresses	No. But indirectly through changes in fracture geometry and transmissivity.	–	–	Yes. Gas pressure could affect the stress conditions in the rock.	Excavation/ operation/ resaturation	Gas flow neglected; minor process.
					Temperate	Neglected; see row Fracture geometry above.
					Periglacial Glacial	Neglected; minor process.
Matrix minerals	No. Mineral composition does not affect flow.	–	–	No. But indirectly through groundwater composition, but insignificant effect for relevant gases.	–	–
Fracture minerals	No. Mineral composition does not affect flow.	–	–	No. But indirectly through groundwater composition, but insignificant effect for relevant gases.	–	–
Groundwater composition	Yes. If groundwater contains dissolved gas, this could come out of solution if the pressure falls, and contribute to gas flow.	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above) except for resaturation phase. No repository generated gas.	Yes. Constituents transported in gas phase may dissolve in water.	Excavation/ operation/ resaturation	Gas flow neglected; minor process (see also Section 5.10).
		Temperate	Neglected; minor process.		Temperate	Gas flow neglected; minor process (see also Section 5.10).
		Periglacial Glacial	Neglected; minor process.		Periglacial Glacial	Gas flow neglected; minor process (see also Section 5.10).

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Gas composition	Yes. Gas composition affects gas phase flow properties (but insignificant).	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above) except for resaturation phase. No repository generated gas.	Yes. Preferential transport of different gas constituents (e.g. because of different partitioning into the water phase).	Excavation/ operation/ resaturation	Gas flow neglected; minor process.
		Temperate	Neglected; main gas generated is hydrogen.		Temperate	Neglected; main gas generated is hydrogen.
		Periglacial Glacial	Neglected; minor process.		Periglacial Glacial	Neglected; minor process.
Structural and stray materials	Yes. Grouting can affect gas escape from the repository.	All	Neglected; gas flow is a minor process.	No. Does not affect structures and materials	–	–
Saturation	Yes. Gas permeability depends on saturation through relative permeability.	Excavation/ operation/ resaturation	Gas flow not modelled explicitly (see row Temperature above). No repository generated gas.	Yes. May alter saturation.	Excavation/ operation/ resaturation	Process neglected in calculations of inflow to tunnels.
		Temperate	Considered in estimates of the capability of the geosphere to transport gas /Hartley et al. 2006a/.		Temperate	Not made explicit in scoping calculations of gas transport /Hartley et al. 2006a/.
		Periglacial Glacial	Neglected; minor process.		Periglacial Glacial	Neglected; minor process.

Temperature in the bedrock. In principle, gas flow affects temperature in the bedrock because heat is transported by flowing gas. However, the heat capacity of gas is low and the rocks at depth in Sweden have low permeability and low porosity, and so the heat transported by flowing gas is negligible in comparison with that transported by conduction through the rocks (see Section 2.1.1 and Section 3.1). The temperature in the bedrock affects the gas flow through the effect of temperature on the viscosity and density of the gas.

Groundwater flow. If both gas and groundwater are present in the pores and fractures in the rock, the flows of gas and groundwater are coupled. In the unsaturated region extending down from the surface, it is not necessary to model the flow of gas because the pressure in the gas phase is very close to atmospheric because the gas is very mobile. Indeed, in most cases, it is adequate to treat the water table as a free surface. Even during the excavation/operation/resaturation period, it is still adequate to model only the flow of the groundwater with the water table represented as a free surface.

Groundwater pressure. The groundwater pressure is an important factor in gas flow. Gas can only enter initially water-filled fractures (and rock matrix pores) if its pressure is greater than the groundwater pressure by an amount that is inversely proportional to the fracture aperture or pore size. It is not expected that gas would enter the matrix pores in Swedish bedrock in general, because of capillary forces.

Repository geometry. Gas flow does not affect the repository geometry. The repository geometry affects the gas flow because the backfilled tunnels and surrounding EDZ may provide permeable paths through the rocks and additional connections between the fractures.

Fracture geometry. If the gas pressure rises sufficiently, this could lead to extension of existing fractures or even the creation of new fractures. The fracture aperture, geometry, and connectivity are key properties that determine how permeable the rock is and so play a major role in determining the gas flow. The fracture aperture is also a key control on the capillary pressure, which determines the excess pressure (above the groundwater pressure) required for gas to displace water from a fracture.

Rock stresses. If the rock is sufficiently impermeable to prevent gas generated in the repository from migrating away from the repository, it is possible that the gas pressure could rise sufficiently to affect the stresses in the rock (and even lead to fracturing). Changes to the rock stresses would affect the properties of the fractures, in particular the aperture and hence transmissivity and capillary pressure. However, the changes to the rock stresses are expected to be small except for the changes due to repository construction and resaturation, ice-loading (on long timescales), tectonic effects (on very long timescales) and earthquakes.

Matrix minerals. In principle, gases could indirectly affect matrix minerals, through their effect on the composition of groundwater flowing through the fractures which can affect the composition of the groundwater within the rock matrix and hence may lead to precipitation or dissolution of minerals within the matrix. However, for the gases of interest, these effects are negligible. Matrix minerals are not expected to affect gas flow for relevant minerals.

Fracture minerals. In principle, gas flow could indirectly affect fracture minerals, through its effect on the groundwater composition and hence on rock-water interactions. However, the effects are considered to be negligible for the gases of interest.

Groundwater composition. Gas flow affects the groundwater composition because gases may dissolve in the groundwater. The groundwater composition may affect the gas flow because dissolved gases may come out of solution if the pressure falls sufficiently.

Gas composition. Gas flow can affect the gas composition because different gases may migrate differently. In particular, they may partition differently between the gas and groundwater phases.

Structural and stray materials. Gas flow would not affect structural and stray material (such as grout used to seal fractures). As the grout degraded over time the permeability of the grouted rock would increase. Grouting in the vicinity of the tunnels would reduce the permeability of the rocks locally and affect the gas flow. It is likely that grouting would be focused on transmissive features, and so the local flow would be significantly affected.

Saturation. Gas flow would affect the saturation. Changes to the saturation as a result of changes in the level of the water table would correspond to flow of air between the rocks and the atmosphere. However, in practice, this would not be explicitly modelled (even for the period of excavation/operation/resaturation) but simply the pressure in the gas taken to be atmospheric, because gas flow would remove any pressure differences in the gas very rapidly.

3.2.3 Boundary conditions

The flow of repository generated gas is mainly determined by the gas production rate and the hydrostatic and gas pressures at the repository depth (and between the repository and the surface). These are the principal factors that will determine in what form the gas will be present (dissolved or as a free gas phase). Gases initially present in the repository when it is closed, and the reduced pressure in the repository at that time, are expected to have only a short-term effect on repository evolution, any effect that they might have being dissipated by the time that the repository has become resaturated.

3.2.4 Model studies/experimental studies

Experiments relevant to gas migration in fractured rock that is initially saturated have been conducted both in the laboratory environment and in the field. Field studies have, for example, been conducted at the Äspö HRL /Jarsjö 1998/, at Grimsel /Finsterle and Pruess 1995/, at Reskajeage /Lineham et al. 1996/, and at Manitoba /Gascoyne and Wushke 1997/. The results of laboratory studies on a variety of natural, artificial and idealised fracture systems are reported in, for example, /Jarsjö 1998/, /Persoff and Pruess 1995/, /Swanton et al. 2003/ and /Hoch et al. 2003/ Theoretical studies relevant to two-phase flows in fracture networks have also been carried out by a number of authors. References to some of these and to other experimental studies can be found in /Rodwell 2000/.

Calculations that have been performed by /Wikramaratna et al. 1993/ show that it is likely that the geosphere has a large capacity to transport gas from the repository up to the surface compared with the rate at which gas is expected to be generated in a repository for spent fuel in copper canisters. Provided, therefore, that the natural fracture system is adequately connected, it is expected to constitute a rapid transport pathway for the gas.

The modelling study by /Painter and Sun 2005/, shows that many issues arising during the period when the repository is open can be analysed without recourse to full two-phase flow modelling. Specifically, maximum and steady-state inflows to an open repository can be predicted without major errors as long as an unconfined aquifer (free-surface model) of groundwater flow is adopted. Hence, the modelling of the open repository period performed in SR-Site /Svensson and Follin 2010a/ considers saturated flow beneath a free surface. An indication of timescales for the resaturation of the repository tunnels after backfilling and closure is of interest. However, it is not thought likely that a field-scale two-phase flow calculation of gas migration from a spent fuel canister through the geosphere will be appropriate (see Section 3.2.8). /Svensson 2010/ estimates the timescales for the hydration process by assuming that the hydration process of the unsaturated parts of the backfill can be modelled as a single-phase, saturated groundwater system with different specific storage for the saturated and unsaturated parts.

3.2.5 Natural analogues/observations in nature

Although attempts have been made internationally to find and use data on flows of natural gases in the geosphere /Rodwell 2000/ in order to develop quantitative predictions of gas migration from radioactive waste repositories, it has not been possible to characterise any such natural systems sufficiently well to provide data that can be used in this way.

There are, however, numerous studies addressing the capability of the geosphere to retain gases, particularly in the field of geological storage of CO_2.

3.2.6 Time perspective

Should a free gas phase pathway form, then the time for gas transport from the repository to the atmosphere would be expected to be much shorter than the time for water transport due to the much lower viscosity. Even, if gas were transported as bubbles the timescales would still be expected to be shorter due to a short vertical pathway under buoyancy and less retention processes. On the other hand, the period over which gas may be generated from defective spent fuel canisters is expected to be considerable.

3.2.7 Handling in the safety assessment SR-Site

Excavation/operation/resaturation period

During the excavation and operation period of the repository, the system is characterised by the tunnels being at atmospheric pressure. Also, the resaturation phase of the repository is included in this period, when the back-filled tunnels go from their initial partial saturation to full saturation.

In a study of the importance of two-phase flow (air-water) in the behaviour of an open repository, /Painter and Sun 2005/ concluded that an unsaturated region may be induced in the vicinity of the tunnels during repository pre-closure operations, and that an unsaturated zone will be formed above the repository. However, for the case considered at Forsmark /Svensson and Follin 2010a/, the formation of these unsaturated regions only had a relatively small effect on inflows to tunnels (compared, for example, to the effect of uncertainty in permeability). An approximation based on saturated groundwater flow using a free groundwater table (unconfined aquifer) is sufficient when steady-state inflows to tunnels, draw downs, and time for resaturation are to be assessed.

The simulations of the excavation, operation and resaturation period are carried out using the DarcyTools program /Svensson et al. 2004, 2010, Svensson and Ferry 2004, Svensson 2004,/. The calculations use a saturated groundwater flow model, with the water table represented by a free surface. Above the surface of atmospheric pressure, DarcyTools models the unsaturated flow using an approximation such that horizontal permeability is reduced outside the free surface. Thus, the effect of gas is taken into account in a simplified manner both for the unsaturated conditions above the water table, and for resaturation of the tunnels.

Temperate climate domain

The issue of main concern to be assessed is whether gas generated in the repository (canisters) can migrate rapidly in a free gas phase through the geosphere and up to the biosphere. The potential consequences of which have been assessed in /Rodwell et al. 2003/. If such rapid migration were to occur it implies that once the gas has escaped through the bentonite buffer around a canister it would not be trapped close to the repository and cause a pressure build up that might modify groundwater flow. It would also imply that, except perhaps in the region of local traps, gas migration pathways will be confined to a very small volume of the rock between the repository and the surface, giving some confidence that any effects of gas migration on groundwater flow and transport will be small.

Scoping calculations of gas generation and migration were carried out for SR-Can /Hartley et al. 2006a, b/. These analyses concluded that probable rates of gas production were sufficiently low that much if not all of the gas could be transported away in solution. If however it is assumed that no gas dissolves, simple estimates show that the gas transport capacity of the fracture network, assuming that it is sufficiently connected between the location of the defective canister and the surface, should be more than adequate to easily transport the gas to the surface without any significant increase in gas pressure in the neighbourhood of the repository. Based on these analyses it is concluded that gas migration is not an issue of concern at the Forsmark site, and that no additional assessment is needed within SR-Site given the similarities in bedrock properties between the hydrogeological model versions used in SR-Can and SR-Site, respectively. The approach in SR-Site then is to neglect gas-phase flow and its influence on water flow in the simulations of the hydrogeology (evolution of salinity and pressure fields) and on the transport of radionuclides dissolved in groundwater.

Periglacial and glacial climate domains

In the assumed evolution of the repository, permafrost[5] and glaciated conditions characterise the climate states existing for a large proportion of the time. The possible impact of climate-related conditions on repository safety in the permafrost and glacial domains is accounted for in the SR-Site Climate report /SKB 2010c/.

As far as gas flow is concerned, the extent of frozen ground is likely to be the most significant climate-related condition. If frozen ground provides a sealing barrier between the repository and the surface, then gas will not be able to escape to the surface but will collect beneath the permafrost. A gas ‘bubble’ beneath the permafrost may then be formed, and water would not be able to flow through the gas bubble. The effect on the groundwater flow would be the same as if the permafrost were slightly thicker. The permafrost would probably not have a horizontal bottom boundary, but there might well be undulations in the bottom surface and migrating gas would tend to collect under domes in the bottom surface of the permafrost. It is also possible that if taliks have formed that some gas might migrate to the taliks and escape. If the thickness of the permafrost increases, it is possible that some gas may become trapped within the permafrost itself. Any gas that had accumulated beneath the permafrost might be released to the biosphere over a relatively short period of time when the permafrost disappears.

If repository temperature is reduced as a result of the development of substantially colder climate states than the one that exists at present, then there could be some reduction in gas generation rates.

The consequences of gas in the geosphere during periods of permafrost and glaciation are not further analysed in SR-Site.

The process of methane ice formation is described in Section 5.11.

Earthquakes

It is considered that gas flow/dissolution is not relevant to the generation of earthquakes, and earthquakes are not relevant generally to gas flow/dissolution, although earthquakes could lead to the sudden release of trapped gas as a result of induced fracturing.

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[5] Permafrost is defined on the basis of temperature as soil or rock that remains below 0°C throughout the year, and may be saturated or unsaturated. If the permafrost is unsaturated it can have significant permeability to gas, but this is unlikely to be the case at the sites under consideration for a repository.

3.2.8 Uncertainties

Uncertainties in mechanistic understanding

There are uncertainties in a quantitative description of gas and two-phase flow through a geosphere in which the rock permeability is provided by a network of discrete fractures. Although it is believed that the basic physics of gas migration is well understood, the application to fractured media involves considerably difficulty. This is fundamentally because the gas migration depends on details of the fracture network, such as fracture aperture variability, and fracture orientation and connectivity, which are difficult to characterise on the scale that controls the properties of the gas pathways. In the terminology of conventional porous medium flow theory, it is difficult to define and characterise the capillary pressure and relative permeability functions for an appropriate elementary representative volume over which these functions can be considered to apply. For a fracture network, these functions cannot be measured in the laboratory in the same way as they can for rock made up of a continuous porous medium (although even here there may be an "upscaling" issue to be addressed).

Model simplification uncertainties in SR-Site

The assessment of gas migration through the geosphere is based on simple arguments about the likely capacity of the discrete fracture network to transport gas compared with the estimated upper bound for the gas generation rate from a defective canister. These arguments consider estimates of the minimum aperture required for gas to dissipate in a free gas phase, and thereby avoid a pressure build up, relative to the minimum aperture of connected open fractures intersecting the deposition tunnels predicted by the DFN model for the site. Estimates of the frequency of connected open fractures intersecting a deposition tunnel are derived with reasonable confidence using DFN models calibrated against hydraulic tests using the Posiva Flow Log (PFL) tool, which also provides estimates of fracture transmissivity. The distribution of transport apertures is then inferred from transmissivity. This last step introduces uncertainty since a general relationships between fracture aperture and transmissivity is difficult establish. However, there is a significant margin between the aperture predicted by DFN models and the minimum for gas flow. Likewise, the disturbance to groundwater flow by a rising stream of gas bubbles is estimated simply by comparing the maximum gas generation rate with the bulk groundwater flow at depth, again estimated from hydraulic tests. Although these simple arguments avoid much of the complexity of actual gas flow channels through rough fractures with variable orientations and interconnections, the approach is robust because the results obtained with cautious assumptions do demonstrate that there is ample capacity in the fracture network to transport all the gas generated from the repository without a pressure build up.

Input data and data uncertainties in SR-Site

Assessment of gas migration behaviour requires an assessment of the likely, or an upper bound to the gas generation rate from defective spent fuel canisters. It also requires sufficient knowledge of the fracture network (e.g. fracture apertures and connectivity) to allow an assessment of the capacity of the geosphere to transport gas. For the gas generation rate, there are sufficient data available to allow a reliable upper bound to be determined. The fracture network characteristics are based on data from a limited number of hydraulic tests and on the use of these and general understanding of relationships between various fracture flow properties to construct computational representations of the fracture network. The latter are evidently rather idealised, and are untested as far as calibration against large-scale gas migration behaviour is concerned. However, some validation is possible by comparison of the results of groundwater flow calculations with field data, and this should provide some confidence that the representation and associated data are reasonable.

3.2.9 Adequacy of references supporting the handling in SR-Site

The references /SKB 2008a, SKB 2009a/, SDM-Site for Forsmark and Laxemar, respectively, are SKB reports that have undergone documented factual and quality review.

The reference /SKB 2010d/, which discusses radiolysis of water and corrosion of iron in a spent fuel canister is an SKB report, produced for SR-Site, that has undergone documented factual and quality review.

The reference /SKB 2010e/, which discusses buffer and backfill processes, rock bolt corrosion and the behaviour of the bentonite is an SKB report, produced for SR-Site, that has undergone documented factual and quality review.

The reference /Painter and Sun 2005/, which discusses the modelling of an open repository, is an SKB report that has undergone documented factual and quality review. However, the SR-Site procedures for review, including formal review protocols, have not been followed; instead, a more free format review was undertaken.

The references /Pruess and Tsang 1990/, which discusses the relative permeability function for a fracture, and /Persoff and Pruess 1995/, which discusses the relative permeability function for a fracture and laboratory experiments, are peer-reviewed articles that have appeared in the open literature.

The references /Mott and Rodwell 1998/ and /Swift and Goodfield 2001/, which discuss the relative permeability function for a fracture, are scientifically consistent with the references /Pruess and Tsang 1990/, /Persoff and Pruess 1995/, and therefore are considered to provide additional support for these.

The references /Hartley et al. 2006a, b/, which discusses modelling of groundwater flow and gas flow, are SKB reports, prepared for SR-Can, that have undergone documented factual and quality reviews.

The report /SKB 2010c/, describing climate-related issues, is an SKB report prepared for SR-Site that has undergone documented factual and quality review.

4 Mechanical processes

4.1 Introduction

4.1.1 General

One of the fundamental safety functions of the bedrock is to give the repository's engineered barriers a mechanically stable environment in both the short and long term. This means that the functions of the buffer and the canister should not be altered significantly by deformations in the rock. Another safety function of the bedrock is to retard the transport of radionuclides to the biosphere, which from a mechanical viewpoint means that the retention properties of the rock should not be seriously degraded by large displacements along fractures and fracture zones, or by extensive formation of new fractures.

In general, the Swedish bedrock offers an environment that can protect and secure the repository functions. Sweden's crystalline basement comprises a part of the Baltic Shield that extends from the Kola Peninsula and Karelia through Finland and Sweden to southern Norway. The bedrock at Forsmark is situated inside the Svecokarelian orogen in the south-western part of the Shield. The Forsmark area consists of a crystalline bedrock that formed between 1.9 and 1.8 Ga before present /Stephens et al. 2007/.

4.1.2 Mechanical evolution of the Shield

In simplified terms, the Shield can be described mechanically as an approximately 80–120 km thick plate of elastic material, which is partly brittle and contains the crust in the uppermost 45 km, resting on a viscoelastic mantle. The conditions in the Shield are complex. The effective elastic thickness of the lithosphere varies significantly from east to west (Bouger coherency estimation points to approximately 100 km in central Finland and to about 30 km in southwestern Sweden) /Pérez-Gussinyé et al. 2004/. Crustal thickness behaves similarly, varying from approximately 60 km in central Finland to about 30 km in south-western Sweden /Muir Wood 1993, Juhlin et al. 1998/. The relation between strength and depth depends on the geothermal heat flow and the horizontal strain rate /Milnes et al. 1998/. Therefore, the strength profile, or the rheological profile, is different for a cross-section through the Shield in northern Sweden with small geothermal flows compared with one in south-eastern Sweden, where the geothermal heat flow is greater /Milnes et al. 1998/. The deformation of the Shield under load is further affected by the fact that it is criss-crossed by a number of deformation zones that enable the different parts of the Shield to move relative to each other, for example along the Protogine Zone, which constitutes the boundary of the Sveconorwegian province in the southwest.

The Baltic Shield is currently affected by two large-scale deformation processes; plate tectonics and glacial isostatic adjustment (GIA). The plate tectonic component includes "ridge push" from the west due to seafloor spreading at the Mid-Atlantic Ridge /e.g. Muir Wood 1993/ and compression from the south due to the Eurasia-Africa plate collision /Hakami et al. 2002/. Current tectonic conditions are judged to have been constant for the past two million years /Muir Wood 1995/.

Glacial isostatic adjustment (glacial rebound or land uplift) due to the retreat of the most recent Fennoscandian ice sheet is still ongoing. Fennoscandia has been subjected to eight glacial periods during the last 740,000 years /EPICA community members 2004/ and will probably experience new glaciations in the future /Wallroth 1997/. The most recent glaciation, the Weichselian, persisted for approximately 100,000 years. The growth of an ice sheet cause depression of the Earth's lithosphere under the load and uplift beyond the ice margin (a so called fore-bulge). Approximately 900 m of maximum vertical subsidence is estimated for the Baltic Shield during the last glaciation /Kakkuri 1986/. The timescale for the downwarping, as well as the timescale for land uplift after melting of the ice sheet, depend on the rheological properties of the viscoelastic material in the mantle. Analysis of gravity data indicates that there is approximately 50 m of remaining rebound /Ekman 1991/.

Sea- and lake-level data together with GPS measurements are used to estimate the current motion of the surface of the Baltic Shield. One hundred years of sea- and lake-level data analysed by /Ekman

1996/ indicate a maximum uplift rate of 9.0 mm/year. Continuous GPS data from 1993 to 2006 analysed within the BIFROST project /BIFROST 1996, Lidberg et al. 2010/ in the ITRF2005 No Net-Rotation Eurasia reference frame, shows that the maximum vertical velocity is approximately 11 mm/year and that horizontal velocities in the most rapidly deforming part of the Baltic Shield are between 1.5–2 mm/year. Uncertainties in the BIFROST estimates are now at 0.2 mm/year in the horizontal components and 0.4 mm/year in the vertical. Analysing the 3D velocity field, the data fit models of glacial isostatic adjustment /Lambeck et al. 1998/ with residuals in the order of 1 mm/year /Lidberg et al. 2010/.

As the deformation field in the Baltic Shield is a combination of tectonic and glacial rebound components, so is the strain rate field. Using simple models, /Muir Wood 1993/ showed that the horizontal rebound strain field exhibits extension (at distances up to about 600 km from the ice-sheet centre) as well as compression (at distances between 600 and 1,400 km from the ice-sheet centre) with strain magnitudes on the order of 10^{-9}/year. Analysis of the BIFROST GPS data using a thick plate approach, /Scherneck et al. 2010/ gave similar horizontal extensional rebound strain magnitudes close to the Earth's surface in the central parts of the Shield, i.e. around the Gulf of Bothnia. The model also indicated horizontal compression in the lower part of the 200 km thick plate.

The magnitude of the contribution from tectonics to the intraplate strain field is difficult to estimate and therefore debated. Using geological indicators and Very Long Baseline Interferometry, /Gordon 1988/ estimated intraplate strain rates to $4–6 \cdot 10^{-10}$/year. Intraplate seismicity in North America and Australia suggests strain rates from 10^{-13} to less than $3 \cdot 10^{-9}$/year /Mazzotti and Adams 2005, Sandiford et al. 2004, Anderson 1986/. Using GPS data from intraplate North America, /Calais and Stein 2009/ note that strain rates are below current GPS uncertainties and suggest an upper bound of approximately 10^{-10}/year, after GIA correction. In the BIFROST GPS analysis by /Scherneck et al. 2010/, the residual velocity observations after subtracting the GIA component are used to estimate a strain rate field. Residual strain rates do not exceed $4 \cdot 10^{-9}$/year in the central parts of the Shield and /Scherneck et al. 2010/ attribute most of the residual strain rates to factors such as sparse GPS station coverage and uncertainties in the GIA model predictions. Estimating the tectonic strain rate field in Fennoscandia is hence difficult both due to uncertainties in the velocity estimates and uncertainties in the GIA process.

In addition, /Muir Wood 1995/ argues that most of the ridge-push deformation is absorbed in the Shield's marginal areas, so that the strain that is transferred each year to the interior of the Shield is not greater than 10^{-11}, i.e. a hundredth of the strain due to glacial rebound. Conversely, /Slunga 1991/ claims that at least a hundred times greater strains are transferred to the interior of the Shield and that the deformation is largely accommodated as aseismic displacements on large deformation zones. According to his model, the clear difference in seismicity between the provinces separated by the Protogine Zone in southern Sweden may indicate that the zone, without exhibiting seismic activity of its own, is of importance for the transmission of tectonic deformation.

Data on the current stress field in the south and central parts of the Baltic Shield show clearly the influence of ridge-push /Slunga 1991, Juhlin et al. 1998, Lund and Zoback 1999, Uski et al. 2003/. The data show a strike-slip state of stress with the maximum horizontal stress in the direction NW-SE. In the northern part of the Shield, however, there is no coherent picture of the stress field as of yet. /Muir Wood 1995/ estimates that the current tectonic regime has prevailed for about 2 million years, whereas the character of the state of stress may have persisted for the most part during the past 25 million years.

During a glaciation, the stress evolution in the crust is determined by the shape and temporal variation of the ice cover, the mechanical properties of the lithosphere and the rheology of the underlying mantle /cf. Lund et al. 2009, Wu 2009/. The increase in vertical stress during loading will correspond to the ice load, whereas the horizontal stresses depend also on lithospheric flexure that results from downwarping; horizontal stresses will increase under the ice whereas they will decrease in the fore-bulge region outside the ice margin. Due to the slow viscous response of the mantle, parts of the horizontal stress response lag behind the evolution of the ice sheet. This is especially noticeable at the end of deglaciation, when the vertical load has disappeared, but there is still appreciable horizontal stress from the down-warped lithosphere. The timescale for a glacial cycle, approximately one hundred thousand years, is short in a tectonic time perspective, and it can be assumed that the state of stress is largely restored between glaciations /Muir Wood 1993, Wu 2009/.

The large-scale movements that take place in the Shield, i.e. glacially induced compression- extension cycles and tectonic compression, determine the boundary conditions for the long-term mechanical evolution of the repository host rock. If no, or very little, strain energy release occurs by seismic or aseismic fault motion, the stress changes due to loading can easily be estimated. A tectonic strain rate in the order of 10^{-10}/year would then give a horizontal stress change of up to about 0.5 MPa in one hundred thousand years, taking the modulus of elasticity to be 50 GPa. Large ice sheets might suppress strain release through fault motion, due to the added normal stress from the weight of the ice /Johnston 1987/. Tectonic strain would then accumulate under the ice sheet to be released at the time of deglaciation and could contribute to cause large earthquakes such as those associated with the postglacial faults observed in northern Scandinavia.

4.1.3 Earthquakes

Located far from plate boundaries where seismicity is high, Swedish bedrock displays most attributes of intraplate domains, e.g. low seismicity. Earthquakes in the Swedish part of the Shield mainly occur in the southwest, in the Lake Vänern area, and along the Norrland coast. No earthquakes of magnitude 6 or larger are know in Fennoscandia in historical times /e.g. Husebye 2005/. The largest known historical earthquake occurred in the Mo i Rana region in Norway in 1819 with a magnitude of 5.8 or lower /Huseby 2005/. The largest historical earthquake in Sweden is the magnitude 5.4 Koster (or Oslofjorden) event in 1904 /Bungum et al. 2009/, and the two most recent earthquakes with magnitude above 4 occurred outside Lund in 2008 (M 4.3) and in the vicinity of Skövde in 1986 (M 4.5). An earthquake occurs when strain energy that has accumulated over a long time of slow deformations is suddenly released by shear displacements along a discontinuity. The released energy scales approximately with the seismic moment, which is the product of the area of the displaced surface, the magnitude of the average displacement and the elastic shear modulus of the rock. In terms of seismic moment (and released strain energy) one step on the magnitude scale corresponds to a factor of about 32 /Hanks and Kanamori 1979/. Earthquakes that occur in one of the Earth's tectonically active areas, e.g. Japan, Caucasus or California, can have magnitudes of around 8, meaning that about 350,000 times more energy is released than in the 2008 Lund earthquake.

Since the seismic moment is directly proportional to the area of the displaced surface, and since the maximum possible average displacement cannot amount to more than a fraction of the fault's extent in its own plane, it follows that large earthquakes can only occur on very large faults.

An earthquake can be perceived as a sudden local rupture at an asperity (roughness) that has been increasingly loaded due to elastic deformation /e.g. Scholz 1990/ or by aseismic creep displacement, i.e. stable time-continuous displacement, along surrounding, smoother portions of the fracture plane /Slunga 1991/. The earthquake is triggered when the stress concentration around the asperity or asperities that lock the fault has become sufficiently high to cause rupture. The altered stress state around the fault may lead to new stress concentrations around other asperities, either on the same fault or in a nearby zone. If insufficient strain energy has been released to restore stability in the region, new ruptures can take place in a sequence of aftershocks. An earthquake has both static effects in the form of a permanent deformation and an altered stress field in the area around the ruptured fault, and dynamic effects in the form of mechanical waves that can be propagated long distances in the Earth's crust.

All the mechanical energy input to the Shield does not necessarily have to be released in detectable earthquakes. The seismically released strain energy may be only a small fraction of the strain energy that is continuously cycled due to deformations in different parts of the Shield /Slunga 1991/. Conversely, frequent earthquakes do not necessarily entail the continuous input of equivalent quantities of strain energy due to ongoing large-scale deformations. Small deformations may be sufficient to trigger large earthquakes, so that energy accumulated over long periods of time is released /Muir Wood 1993/.

There are two different views regarding which type of large-scale deformation is the principal cause of the current seismic activity in Scandinavia:

1. Deformation due to tectonic movements, "ridge push".
2. Deformation due to the differential land uplift that is still in progress since the most recent ice age, "glacial rebound".

However, with increasing number of focal mechanism determinations, plate tectonics is shown to be the main driver of seismicity /Slunga 1991, Uski et al. 2003, Bungum et al. 2005/. Furthermore, there is evidence that intense seismic activity, evidenced by postglacial faulting, took place in Lapland in direct conjunction with the melting of the most recent ice cap /e.g. Lagerbäck 1979/. These events are inferred to have reached magnitudes up to 8 /Bungum et al. 2005/. The seismic activity in the area may at some time have been on the same level as that which currently exists in highly tectonically active areas, such as Iran /Muir Wood 1993/.

There are two basic views concerning the mechanism of postglacial faulting.

1. Tectonically generated stresses accumulated during the glaciation and were released in the form of earthquakes when the vertical stresses were reduced in response to retreat of the ice sheet. The reason why postglacial fault displacements took place in this part of the Shield and not at other places is that the glaciation had a longer and unbroken duration here, so that larger amounts of energy could accumulate.
2. The horizontal stresses in the upper crust increased slowly under the weight of the ice because of crustal flexure. When the ice disappeared, part of the glacially induced excess in horizontal stresses remained due to the long response time of the viscous mantle, leaving suitably oriented potential fault planes in a state of instability.

Both views are in accordance with the direction of the fault zones. The question has received a great deal of attention from the geological community, and the prevailing view is that both mechanisms were involved /Stanfors and Ericsson 1993/. /Wu 2009/ and/ Lund et al. 2009/ argue, however, that the tectonic strain rate is too low for mechanism #1 to be important and that mechanism #2 dominated. This does not mean that tectonic compression is unimportant to the extent and scope of postglacial seismicity. On the contrary, the induced instability following the disappearance of the stabilising ice cover is likely to have triggered release of tectonic strain energy accumulated over periods of time much longer than one glacial cycle. This would mean that the large postglacial earthquakes were powered mainly by tectonic stresses, but triggered by endglacial instability. There is also agreement that the fault displacements took place as a reactivation of existing fracture zones rather than new fracturing.

For the safety assessment, the possibility of postglacial faulting following future glaciation cycles is the main concern. Although it is debated whether any significant postglacial faulting took place in areas other than Northern Sweden after the last glaciation /Munier and Hökmark 2004/, (and also whether it happened at all in connection with previous glacial cycles /Lagerbäck and Sundh 2008/), the possibility of future postglacial earthquakes near the repository cannot be excluded.

4.1.4 Repository rock mass

Deformation and strength properties

In a mechanical sense, rock masses are composed of intact rock and different types of discontinuities, i.e. fractures and fracture zones. When the rock mass is subjected to loads of different kinds, there will be both intact rock deformations and fracture deformations. At high loads, fracturing, i.e. failure of intact rock and propagation of existing fractures may occur.

The deformation and strength properties of the rock mass are thus dependent not only on the strength and deformation properties of the constituent rock types, but also on the frequency, orientation and mechanical properties of the discontinuities. Two different methods of determining equivalent continuum rock mass properties are demonstrated in the rock mechanics site descriptive model /Glamheden et al. 2007/. The two methods are based on different ways of processing site data, i.e. by numerical modelling and by empirical estimation. Site data are parameter values of fracture network models and measured values of intact rock properties and fracture properties.

On the tunnel and deposition hole scale, the mechanical strength and deformation properties of the individual rock mass components, i.e. the intact rock and the fractures, are more relevant than the equivalent rock mass properties. To assess and understand the mechanical evolution on different scales, it is necessary to have models and data relevant for the rock mass, for the intact rock and for the discontinuities.

State of stress

The mechanical evolution of the repository starts from an initial state that is controlled by the undisturbed *in situ* stresses. Not only the effects of excavation and construction, but also stress effects of additional future loads and load variations will depend on the *in situ* stress state and on how the geometry of the repository is adapted to it. For Swedish bedrock, it is usually assumed that one of the principal stresses (usually the minor stress) is approximately vertical and corresponds to the weight of the overlying rock, which means approximately 13.5 MPa at 500 m depth. This is valid especially in areas with a low topographical gradient. The major and intermediate principal stresses are then both approximately horizontal. The major horizontal stress is usually oriented NW-SE. The state of stress in terms of magnitude and orientation may be locally affected by heterogeneities such as fractured zones. Both general and site-specific regression relations between *in situ* principal stresses and depth exist, but the variations are great, both between different sites and locally within smaller areas. The site descriptive models include stress-state descriptions based on stress measurement and on results of attempts to capture large-scale mechanisms, e.g. shear displacements along large fracture zones, that are likely to be responsible for observed spatial variations /Glamheden et al. 2007/.

4.1.5 Processes in the safety assessment

All mechanical processes in the host rock have to do with deformations, and all deformations have to do with loads and stresses. These fundamental concepts link together the components of the rock mass, the intact rock and the discontinuities, in such a way that there is no logical and at the same time expedient subdivision of the geosphere's mechanics into individual processes. Fracture propagation, for example, involves at the same time ongoing brittle deformation of intact rock and displacement along an existing fracture. The following subdivision into processes has been made to facilitate the description here:

- Displacements in intact rock.
- Reactivation – displacements along existing discontinuities.
- Fracturing (formation and propagation).
- Creep displacements.

By "displacements in intact rock" is meant the main elastic displacements that occur in rock without visible fractures at moderate loads, i.e. at loads that do not cause failure.

By "reactivation – displacements along existing discontinuities" is meant all types of displacements, elastic and inelastic, shear and normal, that take place along discontinuities of various kinds.

By "fracturing" is meant failure in intact rock, both by formation of new fractures and growth of existing fractures.

All deformations in the repository rock are time-dependent in the sense that all load changes, instantaneous and continuous, are distributed over time. By creep displacements is meant delayed and slow deformations that occur without load changes because the intact rock and the rock fractures have time-dependent material properties. Spalling, i.e. brittle failure in the walls of deposition holes, counts as fracturing, even if there is a time-dependence of the micro-fracture growth and coalescence that eventually result in macroscopic failure.

The rock mass is made up of intact rock and of discontinuities. That is why "displacements in intact rock", "reactivation" and "fracturing" are fundamental and general processes. All load changes are accompanied by displacements in intact rock. If there are suitably oriented fractures, the displacements occur preferentially along them. At large loads, fracturing also sometimes occurs, especially if suitably oriented fractures along which the displacements can take place are not present. "Creep" comprises delayed displacements in intact rock and delayed reactivation and fracturing. Therefore, it is not, strictly speaking, a separate process. It has been deemed expedient, though, to regard the aggregate effect of all types of deformations that are influenced by strain-rate dependence or by material properties that change over time as one special process.

Figure 4-1 shows examples of processes and process interdependencies, cf. also e.g. /Tang and Hudson 2010/. Elastic intact rock deformations create loads on fractures, possibly leading to

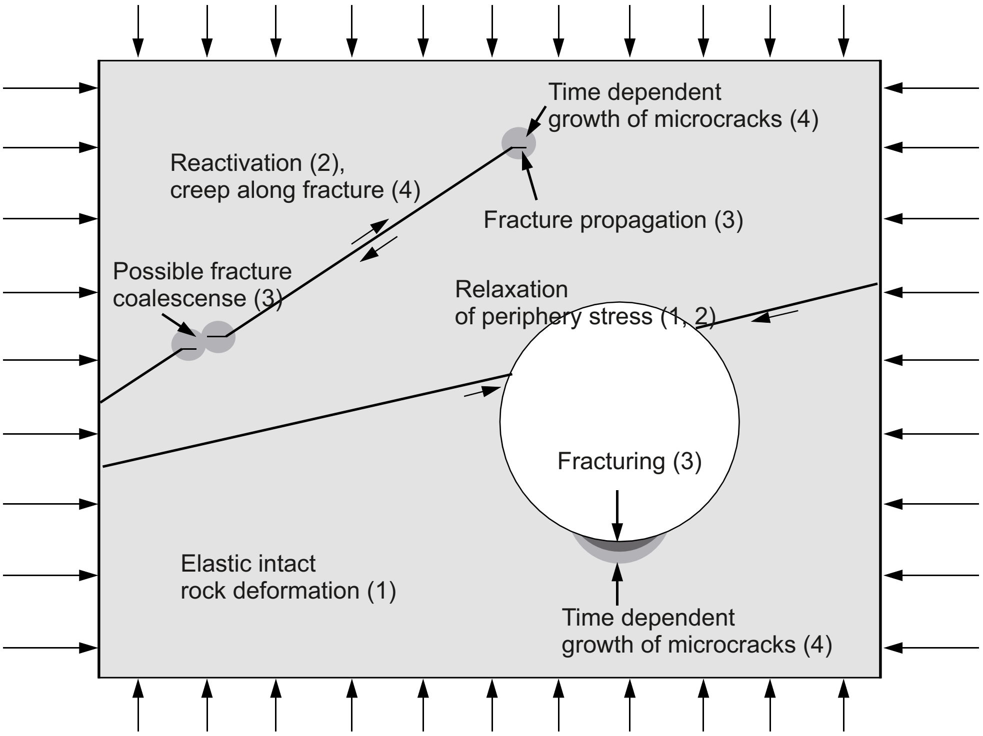

Figure 4-1. *Schematic showing examples of mechanical SR-Site geosphere processes in rock volume under load: Displacements in intact rock (1), Reactivation (2), Fracturing (3) and Creep displacements (4).*

reactivation and slip. Depending on the slip magnitude, there may be time-dependent growth of micro-cracks in regions of stress concentration around the tips of the fracture and, possibly, fracture propagation and fracture coalescence. If the fracture shear stress is sufficiently high there may be a continued slow shear deformation, or creep displacement, along that fracture. Around openings, intact rock deformations lead to high tangential stresses which may cause direct brittle failure close to parts of the periphery where the stress is at maximum and the confining pressure is low. Further out where stresses are high enough to initiate cracks, but below the failure limit, there may be regions of microcrack growth. Deformations associated with time-dependent growth of micro-cracks count as creep displacements in the following text, even if the load causing the crack growth is not strictly constant over time. Similarly, time-dependent fracture displacements count as creep, even if there is shear stress relaxation over time.

4.2 Displacements in intact rock

4.2.1 Overview/general description

No mechanical processes in the geosphere can take place without displacements also occurring in the intact rock. Therefore, the process is fundamental although it does not have any implications on performance and safety in its own right, i.e. without accompanying fracturing and fracture displacements.

In the case of intact crystalline rock, linear-elastic relations valid for isotropic materials are used to approximate stresses and displacements. At a given mechanical load, the displacements are, therefore, determined by two elastic parameters, i.e. Young's modulus and Poisson's ratio. It is recognised that crystalline rock develops micro-cracks at approximately 50% of the peak uniaxial strength. In the repository, these micro-cracks may form locally, but the overall response of intact rock is considered to be elastic. It is anticipated that stresses as high as 50% of the peak strength will be found only locally close to the walls of the repository openings. Elsewhere in the repository, the stress magnitude will be well below the stress level required to cause crack initiation.

When canisters with spent fuel are deposited in the bedrock, the temperature of the rock will increase due to the fuel's residual power or decay heat. For a free volume of intact rock, a uniform temperature increase would result in a volume expansion that depends solely on the coefficient of thermal expansion. Since the rock in the repository is constrained, the expansion is completely or partially suppressed and thermal stresses are generated around the canister holes and the repository. The actual volume expansion and the thermal stresses are dependent on the coefficient of thermal expansion, the degree of confinement and the compression properties of the rock.

4.2.2 Dependencies between process and geosphere variables

Table 4-1 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 4.2.7.

Temperature in bedrock; Temperature changes will give intact rock displacements and thermal stresses because of thermal expansion. Within the temperature range 0–150°C the temperature dependence of the elastic parameters is negligible /Lau et al. 1991/. Within the rock temperature range that can be expected in the repository, the expansion coefficient is approximately temperature independent /Swan 1978/. Rock displacements will have no measurable influence on the temperature.

Repository geometry; The orientation of the tunnels in relation to the *in situ* stress field, the shape and size of tunnels and deposition holes, and the canister spacing have an important influence on the near-field stresses. The canister spacing is important to the thermal stresses in the near field as well as in the far field.

Fracture geometry; The geometry of the fracture system contributes to control the stress field, e.g. because of stress redistribution effects close to slipping fractures. Intact rock displacements alone cannot change geometrical conditions more than very marginally.

Rock stresses; The coupling to the rock stresses is given by approximately linear-elastic stress-strain relations, by the values of the elastic parameters and by the volume expansion coefficient.

Matrix minerals; For given load conditions, the mineral composition determines the mechanical behaviour of the intact rock. The mineral composition influences the elastic properties and the volume expansion coefficient of the intact rock.

Fracture minerals; Fracture minerals influence the mechanical properties of the fractures and can therefore, similar to the fracture geometry, contribute to determine rock stresses.

Table 4-1. Direct dependencies between the process "Displacement in intact rock" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. Determines thermal expansion.	Excavation/ operation	Neglected; little significance compared with impact of stress.	No.	–	–
		Temperate	Temperature evolution is part of thermo-mechanical analyses.			
		Periglacial	Temperature input to stress analyses.			
		Glacial	Neglected; little significance compared with impact of ice load.			
Groundwater flow	No.	–	–	No.	–	–
Groundwater pressure	No. But indirectly through stresses according to effective stress concept.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Gas phase flow	No.	–	–	No.	–	–
Repository geometry	No. But indirectly through stresses.	–	–	No.	–	–
Fracture geometry	No. But indirectly through stresses.	–	–	No.	–	–
Rock stresses	Yes. According to stress-strain relation.	Excavation/ operation	Site-specific rock stresses as input to calculations and zero normal stress at ground surface and peripheries of tunnel openings.	Yes. According to stress-strain relation.	All	Output from calculations.
		Temperate	Thermal stresses calculated in model. Zero normal stress at ground surface.			
		Periglacial	Thermal stresses calculated in model. Zero normal stress at ground surface.			
		Glacial	Stresses at repository depth from ice/crust/mantle model. Otherwise same as for temperate conditions.			
Matrix minerals	Yes. Controls stress-strain relation.	All	Site-specific rock mechanics property data.	No.	–	–
Fracture minerals	No. But indirectly through stresses.	–	–	No.	–	–
Groundwater composition	No.	–	–	No.	–	–
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	No.	–	–	No.	–	–

4.2.3 Boundary conditions

The peripheries of the repository openings and the ground surface are the boundaries of the geosphere for all mechanical processes. Mechanically these boundaries are subject to the same type of boundary condition throughout the entire repository lifetime, i.e. a state of more or less well-defined normal and shear stresses. At the opening peripheries, the normal and shear boundary stresses will both be zero before deposition and backfilling. Some time after closure the normal boundary stress will correspond to the swelling pressure of the bentonite buffer for deposition holes and to the swelling pressure of the backfill for deposition tunnels. The ground surface will be at zero normal stress at all times except for the glaciation period, when the boundary normal stress will vary due to effects of the glacial loading.

4.2.4 Model studies/experimental studies

Results from analyses of elastic and homogenous models of the repository rock mass provide useful information on the mechanical response to excavation, heating etc. /Probert and Claesson 1997/ studied a large-scale repository model with analytical thermo-mechanical expressions. The analysis gave horizontal thermal stresses of about 17 MPa at maximum, i.e. at the repository horizon, some 50 years after deposition. Later, the horizontal stresses decreased in magnitude, and appeared at increasingly larger vertical distance from the repository. At the level of the repository, the vertical stress increased by about 3 MPa with a maximum about 1,000 years after deposition. The analytical results agreed closely with numerical results from a 3DEC model, computed specifically to test the validity of the analytical solution.

/Hökmark 2003/ analysed rock displacements, using 3DEC, caused by tunnel and deposition-hole excavation. Values of rock stresses and rock property parameters used in the analyses were typical of the conditions around the Prototype tunnel in the Äspö HRL. The fracture system was based on a discrete fracture network model established by use of trace data from the walls of the tunnel. All fracture radii were smaller than 10 m. Analyses were performed with and without consideration of the fracture system, i.e. also for the assumption of intact rock only. The results showed that the majority of the displacements were due to intact rock displacement. The contribution from moving fractures was about 30% if the fracture friction angle was 20 degrees and about 20% if the friction angle was 30 degrees. The magnitudes of the displacements were in the order of a couple of millimetres, verifying that intact rock displacement alone will be very small and, hence, cannot have any impact on repository performance and safety. Similar results have been obtained in thermo-mechanical near-field analyses of KBS-3 repositories adapted to the Forsmark and Simpevarp sites /Hökmark et al. 2006/.

Using core samples from the investigated sites, values of intact rock parameters have been determined in the laboratory and reported in the site descriptive models, e.g. /Back et al. 2007, Sundberg et al. 2008a, b, Glamheden et al. 2007, Hakami et al. 2008/. For parameters that are relevant to intact rock displacements, i.e. Young´s modulus, Poisson's ratio and the thermal volume expansion coefficient, values for crystalline rocks do not usually vary over wide ranges. The site investigation data are well within the ranges used in recent and previous modelling work.

4.2.5 Natural analogues/observations in nature

Not applicable.

4.2.6 Time perspective

Intact rock displacements will take place during all repository phases as long as there are changes in the loading/boundary conditions. The change in load will be particularly large and intense in the near field during excavation. After excavation, depending on the *in situ* stresses and the intact rock strength, there may be small regions close to the walls of the deposition holes where crack initiation and possibly brittle failure, spalling, has taken place. During the temperate period, the regions of failure increase in volume because of the thermal load. The horizontal background stresses effective during the glacial load are in the same order of magnitude as those of the early temperate phase /Hökmark et al. 2010/. However, because of the confinement provided to the opening peripheries by the water-saturated bentonite buffer and backfill materials, the volumes of potential failure are smaller. Brittle failure and micro-fracture growth are aspects of the fracturing process and the creep process, and are dealt with in the following sections.

4.2.7 Handling in the safety assessment SR-Site

Excavation/operation period

The contribution made to changes of the geometry of the near field by displacements in intact rock alone is without direct importance for repository safety and performance. However, intact rock displacements are fundamental to the behaviour of fractured rock. The process is included in the near-field modelling of the effects of excavation of tunnels and deposition holes. The results are used to assess the risk for stress-induced brittle failure around the repository openings and to obtain estimates of possible permeability changes caused by shear and normal fracture displacements.

Model; The 3DEC models are described in /Hökmark et al. 2010/.

Boundary conditions; Zero normal stress is assigned at all boundaries (see general boundary condition statement above).

Handling of variables influencing the process; Rock stresses are included in the model. Mineral composition determines values of property parameters and is included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model.

Temperate climate domain

For the near field, the handling is the same as for the excavation/operation period, i.e. it is included in 3DEC stress-deformation analysis of the near field. The mechanical state obtained at the end of that period is used as the point of departure for the simulation of the period with thermal load. The thermal loads are conditioned by the layout established for the different rock domains /SKB 2009b/.

For the far field, the process is modelled with large-scale 3DEC models using thermal loads corresponding to those of the near-field models.

Model; The 3DEC models described in /Hökmark et al. 2010/.

Boundary conditions; Zero normal stress is assigned at the ground surface and at the deposition hole walls, i.e. the swelling pressure from buffer and backfill on the walls of the openings is ignored.

Handling of variables influencing the process; Temperature and rock stresses are included in the model. Mineral composition determines values of property parameters and is included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model.

Periglacial climate domain

The process is modelled using the 3DEC near-field models described for the temperate phase, using temperature data relevant for the periglacial period /Hartikainen et al. 2010/.

Glacial climate domain

The handling is included in the 3DEC stress-deformation analysis of the near field, using the mechanical state obtained at the end of the temperate period as the point of departure.

Models; The 3DEC models described in /Hökmark et al. 2010/.

Boundary conditions; Normal stress is assigned at the ground surface and horizontal stress at repository depth according to the ice/crust/mantle model /Lund et al. 2009/. The swelling pressure from buffer and backfill on the excavation boundaries is ignored.

Handling of variables influencing the process; Rock stresses are included in the model. Mineral composition determines values of property parameters and is included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model.

Earthquakes

The handling is included in the modelling of induced shear displacements, see Section 4.3.

4.2.8 Uncertainties

Uncertainties in mechanistic understanding

There are no conceptual uncertainties in describing displacements in intact rock.

Model simplification uncertainties in SR-Site

The simplifications, if any, are too minor to generate any uncertainties.

Input data and data uncertainties in SR-Site

Parameter values for material properties used in the 3DEC models are based on the site descriptive models. These data are provided in the SR-Site data report /SKB 2010b/.

4.2.9 Adequacy of references supporting the handling in SR-Site

The supporting references /Lund et al. 2009/, /Hartikainen et al. 2010/ and /Hökmark et al. 2010/ are SKB reports that have undergone a documented factual- and quality review.

4.3 Reactivation – displacement along existing discontinuities

4.3.1 Overview/general description

The most significant mechanical process in the geosphere from a repository safety viewpoint is displacements/deformations in large discontinuities. Discontinuities of all types, from millimetre-sized fractures to composite fracture zones extending several kilometres, are mechanical systems whose behaviour is controlled by the loads to which they are subjected, by the prevailing groundwater pressure and by their own inherent mechanical properties. There are two basic types of fracture displacements: normal displacements and shear displacements. However, these two types of displacements often combine into a mixed mode displacement. At repository depth, the shear component is anticipated to be much larger than the normal component for all realistic load cases.

On the near-field scale, and possibly on the tunnel scale as well, large fracture zones hardly appear as discrete discontinuities, but rather in the form of an elevated frequency of individual fractures or as areas with different mechanical properties. On the repository scale, however, it is both customary and computationally adequate to regard large fracture zones as discrete discontinuities. Single fractures in the rock mass outside the large fracture zones contribute to the average properties of the rock mass, but are not represented on the repository scale as individual units. The state of knowledge regarding deformation and strength properties differs considerably for single fractures and large fracture zones.

Normal displacements

Displacements in the direction normal to the fracture can take place due to changes in the effective normal stress (e.g. increased or decreased compression, increased or decreased water pressure in the fracture), and due to far-reaching shear deformations where irregularities force the fracture surfaces to separate (dilatancy).

In the case of pure normal loads, the greater the normal stiffness of the discontinuity, the less mechanical importance the discontinuity has, i.e. the discontinuity tends to be mechanically invisible. In the case of single fractures, the normal stiffness is strongly dependent on the normal stress, which means that the stiffness is large for fractures in high compression and small for fractures in low compression /Barton et al. 1985/, cf. /Fransson 2009/ for additional references. For normal stresses of approximately 10 MPa it can be assumed that the normal stiffness of large zones is around two orders of magnitude smaller than that of single unfilled fractures /Shen and Stephansson 1990a, b/.

In the rock between fracture zones, the fracture density is relatively low, as compared to the interior of fracture zones. This, together with the large normal stiffness and the small mechanical aperture of individual fractures, means that purely normal fracture displacements are generally of little importance for the mechanical properties of the competent rock mass. On the other hand, fracture zones that have small normal stiffness can absorb large compressions and thereby influence the mechanical properties of the rock mass.

Shear displacements

The deformation and strength properties of single fractures are complexly dependent on, among other things, the strength of the material in the fracture surfaces and the topography of the fracture surfaces. /Barton et al. 1985/ proposed empirically based stress-deformation relations for both shear displacements and normal displacements. These relations are based on laboratory determination of values for a small number of fundamental fracture parameters using a standardised procedure. These are the fracture's residual friction angle φ_r, the fracture's surface roughness JRC (Joint Roughness Coefficient) and the fracture's surface strength JCS (Joint Compressive Strength).

Thus, in the case of single fractures, elaborate material models exist. These can be used to describe the type and size of fracture displacements under given loading conditions, provided that the assigned parameter values are representative of the fracture in its entirety. In practice, e.g. in numerical simulation of rock mechanics problems, the parameter values are not known explicitly and estimates have to be used, for example based on comparisons with cases where systematic laboratory determinations have been done. In analysis of displacements of individual fractures in a rock mass, the greatest problem is not that the material properties of the fracture are not known with sufficient accuracy, but that assumptions must be made concerning the fracture's position, orientation, extension and interaction with other fractures. These geometric characteristics are usually more important than details of the fracture properties, which is why simpler and more robust material models are often used in practice. Nevertheless, these simpler models still possess the basic features of more sophisticated models. Figure 4-2 shows a comparison between Barton-Bandis' model for shear displacement /Barton et al. 1985/and an idealised elastoplastic model with a Coulomb failure criterion.

/Olsson 1998/ showed that the elastic part of the deformation can amount to a millimetre or so. Shear displacements of such size that they are of importance for the safety of the repository are controlled by strength parameters, i.e. by cohesion and friction.

For fracture zones, i.e. structures composed of systems of single fractures, the mechanical behaviour is more complex. Zone thickness and fracture frequency, plus amount and type of interaction between constituent fractures, can vary within wide limits for one and the same fracture zone. If the fracture zone is conceived as a discrete discontinuity, mechanical properties that represent the aggregate influence of the constituent fractures must be assumed. No experience similar to that for the description of the mechanical properties of single fractures exists, but when fracture zones are explicitly represented in numerical models, stress-deformation relations similar to those used for single fractures are usually assumed.

4.3.2 Dependencies between process and geosphere variables

Table 4-2 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 4.3.7.

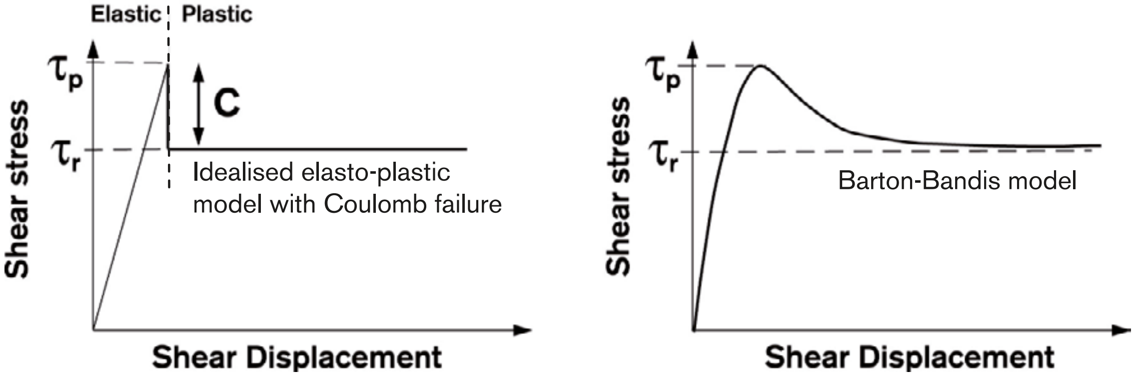

***Figure 4-2.** Stress – deformation relations for single fractures. τ_p = shear stress at failure, τ_r = residual shear strength, c = cohesion.*

Table 4-2. Direct dependencies between the process "Reactivation – displacement along existing discontinuities" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	No. But indirectly via stresses.	–	See Section 4.2.	No.	–	–
Groundwater flow	No.	–	–	No. But indirectly through fracture geometry.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Groundwater pressure	Yes. Effective stress reduction has influence on shear strength.	All	Included in the model as fracture pore pressure.	Yes. But only for rapid displacements.	All	Not considered.
Gas phase flow	No.	–	–	No. But indirectly through fracture geometry.	–	–
Repository geometry	No. But indirectly through stresses.	–	–	No.	–	–
Fracture geometry	Yes. Maximum possible shear displacement depends on fracture size.	All	Generic fracture systems.	Yes.	All	Aperture changes evaluated from fracture stress results.
Rock stresses	Yes.	Excavation/ operation	Site-specific rock stresses. Zero normal stress at ground surface and peripheries of tunnel openings.	Yes.	All	Output from calculations.
		Temperate	Thermal stresses are calculated in the model. Zero normal stress at ground surface and peripheries of tunnel openings.			
		Periglacial	Stresses at repository depth from ice/crust/mantle model /Lund et al. 2009/. Thermal stresses are calculated in the model.			
		Glacial	Stresses at repository depth from ice/crust/mantle model /Lund et al. 2009/. Otherwise same as for temperate period.			
Matrix minerals	Yes. Affects mechanical properties of fracture surfaces.	All	Site-specific rock mechanics property data.	No.	–	–
Fracture minerals	Yes. Affects stress-deformation relations.	All	Site-specific fracture property data.	Yes. Maybe, in case of fracture shear displacements under high normal stress with extensive damage done to asperities.	All	Neglected. The change in mineral composition following a shear deformation is judged to be of minor importance to the mechanical behavior compared to the overall impact of the initial undisturbed composition.
Groundwater composition	No.	–	–	No.	–	–
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	No.	–	–	No.	–	–

Temperature; There are no indications that the temperature dependence of strength of rock fractures is sufficiently large that fracture displacements could be impeded or promoted. The energy expended on friction is too minor to have any influence on the temperature.

Groundwater flow; Groundwater flow variations will not promote or impede fracture displacements. Fracture displacements will give some changes of fracture apertures. This will affect the groundwater flow.

Groundwater pressure; Pressure variations will give normal displacements, i.e. changes in mechanical aperture. In addition, there will be changes in fracture shear strength which potentially may give shear displacements. For fractures in high compression, aperture changes will be small and shear strength reductions will not be significant. For fractures in low compression, both effects may be important. Seismic events, i.e. rapid, large-scale fracture displacements, may create transient pore pressures, whereas fracture displacements caused by time-continuous changes in the load conditions will be sufficiently slow to allow water to move and pressures to keep approximately constant.

Gas phase flow; Similar to groundwater flow, there will be changes in gas flow when fractures move, but no mechanical effects of gas flow variations.

Repository geometry; The geometry (location of individual fractures relative to openings, tunnel orientation relative to *in situ* stress field, spacing between canisters) influences fracture shear and normal stresses, and the scope and extent of fracture displacements. Fracture displacements do not affect the repository geometry.

Fracture geometry; The orientation, size and spacing of fractures are important to the process. The size of a fracture or fracture zone sets bounds to the shear deformation that can occur at a given load. The maximum deformation of a fracture in an elastic medium can be determined analytically /Eshelby 1957/ and is dependent on the extension and friction angle of the fracture and on the elastic properties of the rock. Figure 4-3 (right) shows analytically derived relations between the radius of a circular planar fracture and the shear slip occurring as a result of shear stress increments.

The slip displacements shown in Figure 4-3 are upper bound estimates. Fracture friction, non-planarity and plastic deformations, for instance around the fracture tips, will reduce the slip.

Fracture displacements may cause aperture changes but not change the geometry of the fracture system otherwise than indirectly. If displacements are large, stress concentrations around the fracture tips may be sufficient for fractures to propagate and coalesce.

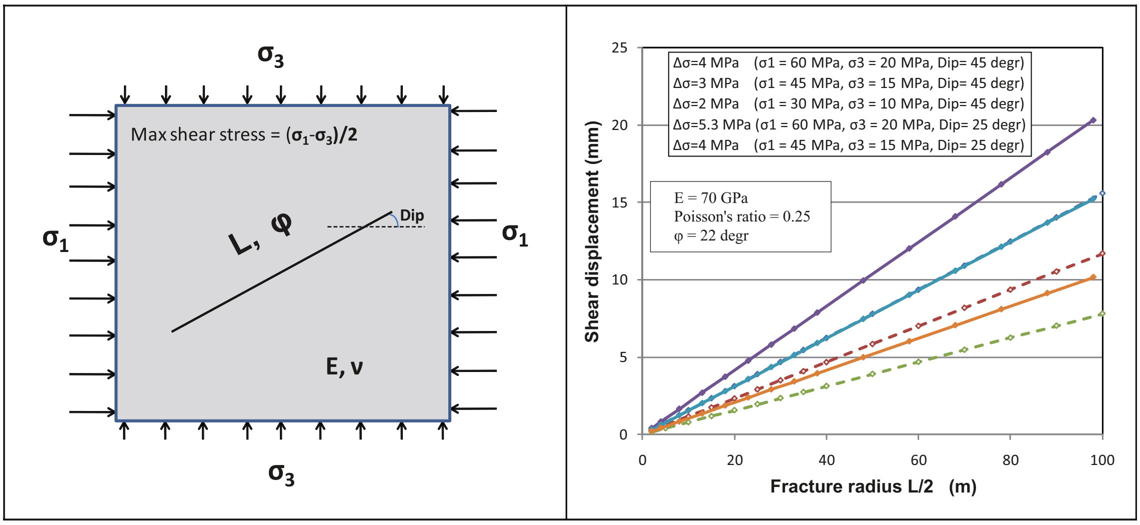

Figure 4-3. *Left: Schematics of fracture of extension L and with friction angle φ in an elastic medium with Young's modulus E and Poisson's ratio ν. Right: Maximum shear displacement on a circular fracture (at the fracture centre) as a function of fracture size for different assumptions of shear load and dip angle. The driving stress Δσ is the fracture shear stress less the friction stress.*

Rock stresses; Changes in fracture shear stress and fracture normal stress are responsible for most fracture displacements. For a given fracture shear load, fractures in high compression typically move less than fractures in low compression.

Fracture shear displacements will create stress concentrations as well as stress-relaxed regions.

Matrix minerals; The matrix mineral composition contributes to determining the mechanical properties of fracture surfaces.

Fracture minerals; The amount and composition of fracture-filling materials have a great impact on the stress-deformation relations of individual fractures. Fracture shear displacements that take place under high normal stress with extensive damage done to asperities may have some influence on the type and amount of fracture-filling minerals.

4.3.3 Boundary conditions

The peripheries of the repository openings and the ground surface are the boundaries of the geosphere for all mechanical processes. Mechanically, these boundaries are subject to the same type of boundary condition throughout the entire repository lifetime, i.e. a state of more or less well-defined normal and shear stresses. At the opening peripheries, the normal and shear boundary stresses will both be zero before deposition and backfilling. Some time after closure, the normal boundary stress will correspond to the swelling pressure of the bentonite buffer for deposition holes and to the swelling pressure of the backfill for deposition tunnels. The ground surface will be at zero normal stress at all times except for the glaciation period, when the normal boundary stress, or boundary pressure, will vary due to effects of the glacial loading.

Earthquakes will generate additional static and dynamic loads.

4.3.4 Model studies/experimental studies

A number of methods exist for numerical analysis of the mechanics of rock masses made up of discrete blocks, for example DEM (Distinct Element Method) and DDA (Discontinuous Deformation Analysis). Overviews are given by /Jing 2003/ and /Jing and Stephansson 2007/. Several rock mechanics studies of displacements and stresses within and around the deep repository have been done with the DEM programs UDEC (2D) and 3DEC (3D). These studies have been carried out on both tunnel and repository scales.

Tunnel scale

/Johansson et al. 1991/ performed thermomechanical calculations with UDEC and 3DEC for a hypothetical repository in the Finnish bedrock. The maximum shear displacements amounted to 3 mm. /Hökmark et al. 2006/ analysed 3DEC near-field models of repositories sited in Simpevarp and Forsmark, using data from draft versions of the preliminary site descriptive models /SKB 2005a, b/, and with layout rules from the underground design premises issued for the deep repository /SKB 2004a/. The 3DEC simulations related to the excavation/operation phase, the temperate phase and the advance and retreat of an ice sheet during a glacial period. Shear displacements amounted to about 3 mm at maximum. At the intersection with the tunnel floor, the displacement was larger, about 5 mm locally, for one particular horizontal fracture. /Hökmark et al. 2010/ analysed the thermomechanical near-field evolution at Forsmark assuming canisters to be positioned according to Layout D2 /SKB 2009b/ and with thermal and thermomechanical rock data according to the site descriptive models established for Forsmark /Back et al. 2007, Sundberg et al. 2008b, Glamheden et al. 2007/. Shear displacements along large fractures intersecting the near-field were not much affected by the openings, but rather determined by the large-scale background stresses in good agreement with analytical results obtained as illustrated in Figure 4-3.

Repository scale

/Hansson et al. 1995/ analysed stresses and deformations around a hypothetical repository in the Äspö HRL rock mass with 3DEC. The largest shear displacements occurred at a large, 65 m thick, fracture zone. The thermal pulse gave a maximum shear displacement of approximately 2 cm and the following glaciation cycle approximately 8 cm.

/La Pointe et al. 1997/ analysed the effect of occasional earthquakes of different magnitudes at different distances from a hypothetical repository using a fracture network model for the Äspö HRL. The analysis was performed with the Displacement Discontinuity code POLY3D using the pessimistic assumption that the fractures were friction free. For earthquakes of magnitude 6.1 at a distance of 2 km from the repository, the greatest shear deformation in the repository area was around 2 mm (Figure 4-4).

/Fälth et al. 2010/ used the 3DEC code to simulate earthquakes in the magnitude range Mw 5.5– Mw7.5. The main objective was to determine the amount of secondary induced slip on fractures (target fractures) located at different distances from the plane of the earthquake faults. The properties of the target fractures were defined according to data given in the site descriptive models established for Forsmark /Glamheden et al. 2007/. For the earthquake fault, the properties were defined as needed to control the fault rupture without regard to actual fault properties. The study verified that earthquake magnitude is not decisive for the response, i.e. induced shear displacements, of nearby fractures, whereas stress drop and fault slip velocity are. The study also showed that fracture slip scales with fracture size, as illustrated in Figure 4-3, also for dynamic loads. At the smallest fault-target distance tried in the study (200 m) the maximum induced displacements were a little less than 50 mm for 300 m diameter target fractures. All target fractures were modelled as perfectly planar circular features.

/La Pointe et al. 2000/ studied how the slip magnitude is influenced by fracturing around the tips of the slipping fracture. As soon as the fracture has slipped sufficiently to initiate propagation around the tips, the fracture will use most of the strain energy to propagate rather than to slip. This means that fracture propagation reduces the slip magnitudes very significantly. Although the study was conducted using fracture propagation criteria derived from results of laboratory tests made on gypsum replicas and without account of the geometry change following fracture propagation, the conclusions point to the possibility that there is a safety margin to all slip estimates based on elastic rock mass models, e.g. /La Pointe et al. 1997/ and /Munier and Hökmark 2004/.

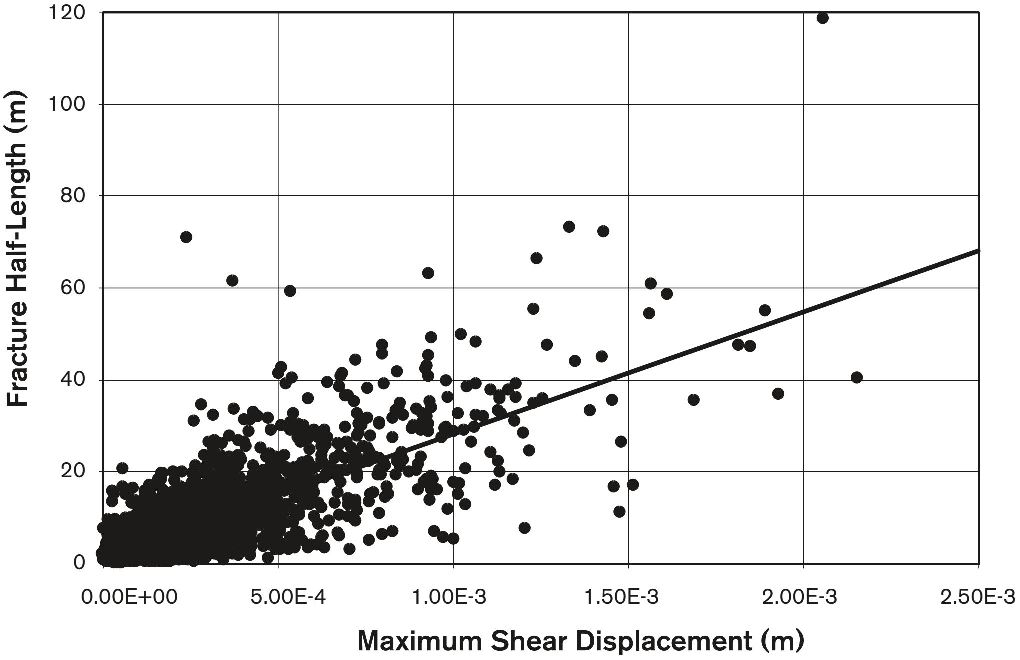

***Figure 4-4.** Shear displacement of fractures in the repository caused by an earthquake of magnitude 6.1 at a distance of 2 km from the repository as a function of the length of the fractures. The scatter around the regression line is due to the distribution in distances of the individual fractures from the earthquake and their distribution in orientation /La Pointe et al. 1997/.*

4.3.5 Natural analogues/observations in nature

In the international literature, as well as in SKB's studies, reports and compilations are found that document observed displacements in the field. A relatively modern database exists that deals with displacement in conjunction with earthquakes /see La Pointe et al. 1997 after Wells and Coppersmith 1994/. The earthquake database contains compilations for different types of faults (Figure 4-5). It can be seen from Figure 4-5 that the relation between maximum displacement and fracture size is of the same type as the theoretically derived relation shown in Figure 4-3.

SKB has studied neotectonics and postglacial faulting at several locations of which the most impressive are located at Lansjärv and Pärvie, Northern Sweden /Stanfors and Eriksson 1993/. The structures containing the postglacial faults are interpreted to be very old (hundreds of millions of years) and their extension in length can be followed over hundreds of kilometres. The fault displacements are considered to be caused by reactivations in already existing structures. The maximum displacements amount to 5 to 10 m (see further /Bäckblom and Stanfors 1989, Stanfors and Ericsson 1993/). Similar observations have been made for normal faults in Hanöbukten and in the North Sea, interpreted from marine seismic investigations (see /Wannäs and Flodén 1994, Muir Wood 1995/).

Other studies are based on observable displacements of geological structures (e.g. shorelines) or fossils that cross faults. A special study of slip along individual fractures, e.g. small faults, has been carried out on outcrops of Ordovician limestone on Öland /Milnes and Gee 1992/. Using orthocerids (fossils) as markers, /Milnes and Gee 1992/ mapped faults ranging between 10 and 100 m, and recorded a maximum cumulative displacement of approximately 10 cm.

In summary, it can be concluded that clear correlations exist between the measured shear displacement and the lengths of the structures on which these displacements have taken place.

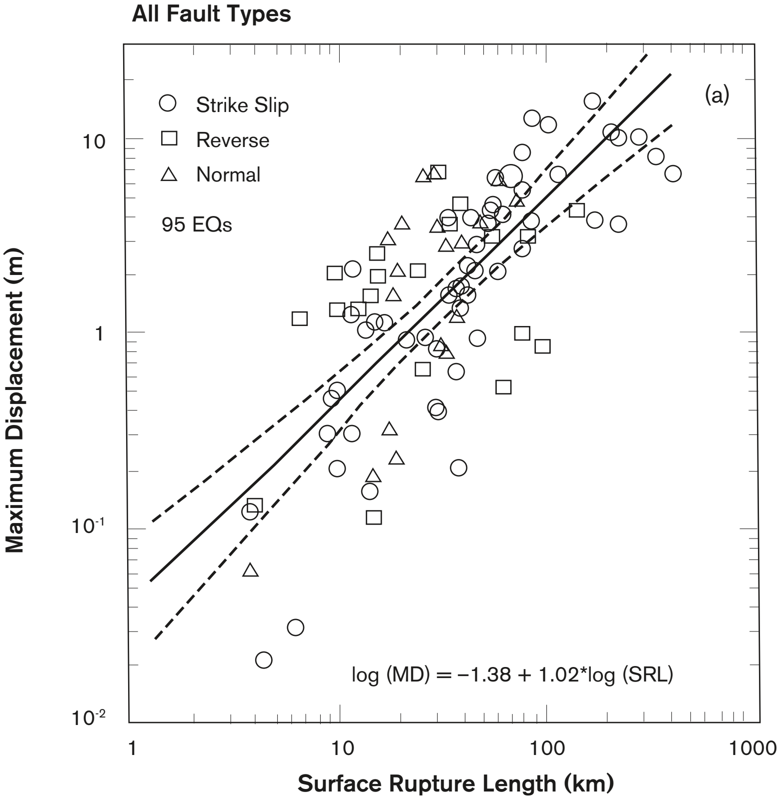

Figure 4-5. *Empirical relation between maximum displacement and observable length of fault structure that has been active in conjunction with an earthquake. The database consists of 95 earthquakes (from /La Pointe et al. 1997/).*

4.3.6 Time perspective

The process will take place as long as there are load changes and changes in ground water pressure. After the thermal pulse, i.e. after some 5,000 years, there are no systematic load changes or changes in groundwater pressure other than those induced by future glacials. Large-scale tectonic strain, i.e. ridge push, may cause continuous aseismic deformations along large deformation zones but no significant changes in the stress state (cf. Section 4.1.2). Seismic displacements of any significance are expected mainly in connection with glaciations, i.e. similar to the way postglacial faulting took place in northern Sweden after the last glaciation.

4.3.7 Handling in the safety assessment SR-Site

Excavation/operation period

The process is modelled in 3DEC studies of stress redistribution effects in fractured near-field rock. The results are used to estimate possible permeability changes caused by shear and normal fracture displacements.

Model; The 3DEC models described in /Hökmark et al. 2006/ and in /Hökmark et al. 2010/.

Boundary conditions; Zero normal and shear stress assigned to all boundaries (see general boundary condition statement above).

Handling of variables influencing the process; Groundwater pressure, fracture geometry and rock stresses are included in the model. Mineral composition and fracture minerals determine the values of property parameters and are included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model. Aperture changes are evaluated from fracture stress results to find possible impacts on fracture transmissivities. Effects on groundwater pressure are not addressed. Effects on fracture minerals (possibly increased amounts) are not considered.

The degree of excavation-induced seismicity is assessed by considering observations of seismicity induced by mining in highly stressed rock at great depths. The excavation activities may, in theory, induce seismicity in the form of fault slip. Of particular concern would be if such seismic events could impair the integrity of the already deposited canisters, i.e. if the fault slip triggered by the excavation activities were larger than 0.05 m. According to regression relations given in /Wells and Coppersmith 1994/ a slip of 0.05 m would require an induced earthquake of approximately magnitude 5. To host such an earthquake, the structure must have a rupture area exceeding a square kilometre. It is unlikely that such a structure would remain undetected after tunnel mapping, which enables us to avoid the structure during deposition. In addition, there is no evidence that present-day deviatoric stresses in Swedish bedrock at repository depth are sufficient to power seismic events of magnitude 5. The largest seismic events recorded in very deep mines in South Africa, for instance, where stresses are high and where the areal extraction ratio (the fraction of horizontal cross section area taken up by openings) is much higher than it will be in the deep repository, are less than magnitude 5 /Munier and Bäckblom 2002/.

Because of the above, the possibility of excavation-induced seismicity is not considered in SR-Site.

Temperate climate domain

The process is modelled in 3DEC studies of thermal load effects. The results are used to estimate possible permeability changes caused by shear and normal fracture displacements. The potential for canister damage because of thermally induced shear displacements along large canister-intersecting fractures is assessed using observations from previous modelling work particularly performed to address this issue. Estimates of the probability of earthquakes during the period are made using literature-derived magnitude-frequency relations. For earthquake consequences, see below.

Model; The 3DEC models described in /Hökmark et al. 2006/ and /Hökmark et al. 2010/.

Boundary conditions; Zero normal and shear stress is assigned at the ground surface and at the walls of the openings. In some of the detailed near-field models analysed in /Hökmark et al. 2006/, however, the swelling of buffer and backfill on the peripheries of the deposition holes and the deposition tunnels is included for completeness.

Handling of variables influencing the process; Groundwater pressure, fracture geometry and rock stresses are included in the model. Mineral composition and fracture minerals determine the values of property parameters and are included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model. Aperture changes are evaluated from fracture stress results. Effects on the groundwater pressure are not considered. Effects on fracture minerals (possibly increased amounts) are not considered.

Periglacial climate domain

The process is modelled using the 3DEC near-field models described for the temperate phase, provided that thermal load cases are identified that indicate that the mechanical state will be changed more than marginally during permafrost. The probability of earthquakes during the period is estimated. For earthquake consequences, see below.

Glacial climate domain

The process is modelled in 3DEC studies of ice-load effects, using stresses obtained from ice/crust/mantle models /Lund et al. 2009/ as boundary conditions. The results are used to estimate possible permeability changes caused by shear and normal fracture displacements. The potential for canister damage because of ice-load induced shear displacements along large canister-intersecting fractures is assessed, using general relations between fracture size and maximum possible shear displacement. The potential for hydraulic jacking, i.e. for fracture-normal effective stresses to drop to zero because of high pore pressures, is assessed from analytical and numerical estimates of pore overpressures associated with advancing, stationary and retreating ice sheets /Lönnqvist and Hökmark 2010/. The probability of earthquakes of magnitude ≥ 5 occurring within 5 km radius from the centre of the Forsmark site in connection with deglaciation is estimated using size/frequency relations derived from the literature. For handling of earthquakes, see below.

Model; The 3DEC models described in /Hökmark et al. 2006/ and /Hökmark et al. 2010/. For earthquake consequences, see below.

Boundary conditions; Boundary stresses according to stress evolution obtained from analyses with the ice/crust/mantle model /Lund et al. 2009/.

Handling of variables influencing the process; Groundwater pressure, fracture geometry and rock stresses are included in the model. Mineral composition and fracture minerals determine the values of property parameters and are included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model. Aperture changes are evaluated from fracture stress results. Effects on the groundwater pressure are not considered. Effects on fracture minerals (possibly increased amounts) are not considered.

Earthquakes

The relevant issue regarding earthquakes is the possibility of induced, secondary slip on fractures that intersect canisters some distance away from the fault generating the earthquake /Munier and Hökmark 2004, Fälth and Hökmark 2007, Fälth et al. 2010/. If that slip exceeds 0.05 m, intersected canisters count as damaged.

Critical radii, i.e. the radii of fractures that potentially could slip in excess of the 0.05 m canister damage threshold when subjected to the effects of a nearby earthquake, have been calculated by /Fälth et al. 2010/ by use of dynamic three-dimensional simulations of events with moment magnitudes ranging between Mw5.5 and Mw7.5. The simulated earthquakes were all high stress drop events that released the largest amount of strain energy consistent with the dimensions of the fault rupture area. Additionally, the fault slip velocity of the synthetic earthquakes was on par with the highest slip velocities ever recorded for real earthquakes, cf. Chi-Chi, Taiwan 1990 earthquake /Ma et al. 2003/, meaning that the dynamic impact on the surrounding rock was significant. All faults ruptured in reverse mode as expected for typical endglacial earthquakes.

Given the high stress drop, high slip velocity representation of the numerically simulated earthquakes, the critical radii depend on the size of the earthquake fault and on the distance to the fault plane. Based on the stress evolution projected by /Lund et al. 2009/ for a future glacial cycle, assumed to be a repetition of Weichsel, and on *in situ* stress models proposed by /Fälth et al. 2010/, five Forsmark deformation zones located within a relevant distance range from the canisters have been identified as potentially unstable in endglacial type stress fields /Fälth et al. 2010/.

The number of critical canisters, i.e. canisters expected to be sheared 0.05 m or more because of seismic events, associated with each of the five deformation zones has been determined by use of methods devised by /Munier 2010/. That number depends on the Discrete Fracture Network (DFN) model assumed to apply to the repository host rock, and on the efficiency of the FPI criterion used to detect and avoid large fractures /Munier 2010/. The method also accounts for the probabilistic nature of the slip distribution among the fractures, i.e. some fractures slip much less than others even if they are of the same size and located at the same distance from the fault. It also accounts for the distribution of slip along the plane of the individual fracture, with the maximum slip at the fracture centre and zero at the tips. The highest number of critical canisters, N1, i.e. the number associated with the most unfortunately located potentially unstable zone and with the most unfavourable DFN model, is used in the calculation of the number of canisters expected to be sheared ≥0.05 m during the next million years. A relevant measure of the frequency of earthquakes of Magnitude ≥5 is derived from available statistics, relevant to present-day conditions in Sweden, as described below.

Earthquake frequencies are given as events per year within circular areas of 5 km radius. At Forsmark, a 5 km radius circular area around the repository includes 36 deformation zones large enough to host an earthquake of Magnitude 5 or larger. Out of these zones, 30 are oriented such that they should count as potentially unstable, meaning that the frequency given for the circular area can be translated to a frequency valid for individual zones. Using frequencies proposed by /Bödvarsson et al. 2006, Table 4-3/ rescaled to an area of radius 5 km, the yearly frequency f is $7.8 \cdot 10^{-8}$ for each of the 30 zones. For the repository the relevant measure is the total frequency $5f$ of earthquakes of Magnitude ≥5 on the five zones found by /Fälth et al. 2010/ to be located closely enough to reactivate fractures within the Layout D2 deposition areas. This gives, using the area frequency proposed by /Bödvarsson et al. 2006/ as an example, $5f = 5 \cdot 7.8 \cdot 10^{-8} = 3.9 \cdot 10^{-7} \cdot \text{year}^{-1}$.

For values of t within the 1,000,000 year assessment time frame, the probability $P1(t)$ that an earthquake of magnitude 5 or larger within a relevant region around the repository (i.e. on any of the five zones) has occurred after time t can be reasonably approximated by Equation 4-1.

$$P1(t) = 5f \cdot t \tag{4-1}$$

For large values of t, Equation 4-1 will overestimate the probability. Provided that earthquake occurrence can be described as a Poisson process, Equation 4-2 gives the probability that exactly one earthquake has occurred after time t. The exponential factor reduces the probability significantly for large values of t.

$$P1(t) = 5f \cdot t \exp(-5f \cdot t) \tag{4-2}$$

Assuming the frequency f to be as suggested above, i.e. $7.8 \cdot 10^{-8} \cdot \text{year}^{-1}$, the probability $P1(t)$ of one potentially damaging earthquake after different periods of time will be according to Table 4-3 for the two approaches above (Equation 4-1 and Equation 4-2).

If there is a period of increased local stability after the strain energy release following an earthquake, earthquakes within the Forsmark region do not occur independently of each other, meaning that the exponential damping in Equation 4-2 is not fully relevant. Therefore the approximate expression (Equation 4-1) is used.

The frequency estimates used to arrive at the probabilities in Table 4-3 are based on statistics that include seismic events occurring in a broad depth range (0 – ≈ 50 km). A magnitude 5 earthquake in Sweden would normally be expected to occur at a depth of about 20 km /Bödvarsson et al. 2006/, i.e. on zones that would not be included in the set of 30 Forsmark zones used to establish the frequency f. This means that the frequency f is overestimated, at least for the 1,000-year assessment time, when seismicity will be determined by the observed depth distribution of earthquakes. For the 1,000-year assessment time frame, the frequency is reduced by 50% as an approximate way of disregarding non-relevant earthquakes in the lower crust. The total probability for one earthquake on any of the five zones at Forsmark is then $P1(1{,}000) \approx 2 \cdot 10^{-4}$.

Table 4-3. Probability P1 of one earthquake after different periods of time at Forsmark for two different probability models.

Probability model	**Time *t***		
	1,000 years	**120,000 years (≈ glacial cycle)**	**1,000,000 years (max assessment time)**
Linear approximation (Equation 4-1)	$3.9 \cdot 10^{-4}$	$4.7 \cdot 10^{-2}$	$3.9 \cdot 10^{-1}$
Exponential factor (Equation 4-2)	$3.9 \cdot 10^{-4}$	$4.5 \cdot 10^{-2}$	$2.6 \cdot 10^{-1}$

For the 120,000-year and 1 million year perspectives, however, there is a possibility that strain energy release and seismicity will indeed be concentrated on faults that break the ground surface because of the nature of the near-surface loading-unloading disturbances commonly assumed to trigger end-glacial earthquakes /Lund et al. 2009, Fälth et al. 2010/. The probabilities P1(120,000) and P1(1,000,000) given in the top row of Table 4-3 are, therefore, pessimistically used without modification.

The maximum number of canisters sheared ≥ 0.05 m after a time *t* as a result of one earthquake is finally obtained as N1·P1(t).

The possibility of an additional large earthquake shortly after the first one, for instance during the same period of endglacial instability, is ruled out because of the extensive strain energy release and the subsequent improved stability found up to at least 2 km away from the first earthquake /Fälth et al. 2010/. The main process that would contribute to restore the stresses within stress-relaxed and stabilised regions around faults that slipped in the past is tectonic compression. Much of the large-scale tectonic compression across the Fennoscandian Shield can be assumed to be absorbed aseismically in large regional fracture zones /Slunga 1991/, which means that the strain rate $\dot{\varepsilon}$ effective for restoring the local stresses can be assumed to be smaller than the large scale strain rate. Estimates of large-scale tectonic strain rates range between 10^{-12} year^{-1} /Muir Wood 1995/ and $1.5 \cdot 10^{-9}$ year^{-1} /Slunga 1991/. Selecting 10^{-10} year^{-1} as a likely upper bound local strain rate estimate (cf. discussion below) and assuming the deformation modulus E of the upper crust to be 64 GPa /Lund et al. 2009/, it follows from Equation 4-3 that it would take some 500,000 years to increase the major horizontal stress by $\Delta\sigma = 3$ MPa. According to the results given in /Fälth et al. 2010/, this is approximately the amount of stress needed to bring the local stress field back to initial undisturbed conditions for which a new glacially-induced loading-unloading cycle would be able to trigger a second large earthquake.

$$t_s = \Delta\sigma / (\dot{\varepsilon} \cdot E) \qquad (4\text{-}3)$$

Here t_s is the stability time, i.e. the time required to restore the stresses after a large earthquake. An important implication of the conditions assumed to control the time-scale for the stress recovery (3MPa required to restore background stress state, a strain rate of $10^{-10} \cdot$year^{-1} and an upper crust deformation modulus of 64 GPa) is that there could be one additional large earthquake within the assessment time frame, but not more. The second earthquake will induce additional slip on fractures that slipped also in response to the first earthquake, meaning that the critical radius will be smaller and that the number of critical canisters will be larger. All slip vectors are pessimistically assumed to be parallel, meaning that the critical radii are reduced by 50% when determining the number N2 of critical canisters after the second earthquake, again using the method described in /Munier 2010/. The second earthquake is assumed to occur on the same fault as the first one, i.e. the one associated with the largest initial number N1 of critical canisters. The number N2 of critical canisters relevant for the second earthquake is pessimistically determined without account of canisters that were critical in the past, i.e. some canisters will count as critical twice.

For $0 \leq t \leq t_s$ the probability of a second large earthquake in the stabilised region is zero. From time $t = t_s$ and onwards, the probability P2(t) of a second large earthquake on any of the five potentially unstable deformation zones can be approximated by:

$$P2(t) = \frac{(5f)^2 \cdot (t - t_s)^2}{2} \qquad (4\text{-}4)$$

Setting, as above, the frequency f to $7.8 \cdot 10^{-8} \cdot$year^{-1} and t_s to 500,000 years gives P2(10^6) ≈ 0.019 for the one million year assessment.

An alternative would be to use the corresponding full Poisson process expression and write (for $t \geq t_s$):

$$P2(t) = \frac{(5f)^2 \cdot (t - t_s)^2 \cdot \exp(5f \cdot (t - t_s))}{2} \qquad (4\text{-}5)$$

This gives P2(10^6) ≈ 0.016. Again, however, the stability period t_s following the first earthquake means that earthquakes occurring in one limited region are not independent events and that the exponential factor may not be fully relevant. Therefore, the probability P2(10^6) of a second earthquake within the one million year assessment period is pessimistically determined by use of Equation 4-4. The number of canisters sheared ≥0.05 m as a result of a second earthquake is obtained as N2·P2.

Yet another possibility of determining the probability of two earthquakes occurring at Forsmark during the one million year assessment time is to recognise that large earthquakes take place preferentially during periods of endglacial instability and that such periods will occur approximately every 120,000 years. Assuming again that it takes 500,000 years to restore the stresses at Forsmark after one large earthquake it follows that the second earthquake cannot occur until four 120,000-year cycles have passed since the first one. Table 4-4 shows the ten possible ways of distributing two earthquakes among the eight endglacial periods. P1 (one cycle) is 0.047 according to Table 4-3. Coloured table entries mean stable cycles. The probability P2(10^6) of a second earthquake within the one million year assessment time is obtained as the sum of the probabilities of the ten discrete cases, i.e. $P2(10^6) = (P1)^2 \cdot [1+2\cdot(1-P1)+3\cdot(1-P1)^2+4\cdot(1-P1)^3] \approx 0.02$.

Table 4-4 concerns the stability case selected for the consideration in SR-Site, i.e. the period of local stability following a large earthquake at Forsmark suppresses the earthquake risk during the three next cycles. Similar schemes can easily be established for other stability cases. For example, if the strain rate effective for restoring the stresses were high enough for one large earthquake every glacial cycle (i.e. $\dot{\varepsilon} \geq 4\cdot10^{-10}\cdot\text{year}^{-1}$, cf. Equation 4-3, giving a stability time of about 120 ka) there would be 28 discrete cases giving a total probability $P2(10^6) = 28\cdot P1^2\cdot(1-P1)^6 \approx 0.04$.

Table 4-4 also illustrates the way the probability of a second earthquake increases over time for the selected stability case (500 ka); there is one case (out of ten) with a second earthquake at time 600 ka, two cases at time 720 ka, three cases at time 840 ka and four cases at time 960 ka. The way the probability P2(t) increases from zero at t= 600,000 years to 0.02 at t = 1,000,000 years time is illustrated in Figure 4-6 (right) along with corresponding results obtained using Equation 4-4 and Equation 4-5. The corresponding probability evolution for the case of a stability period of 120 ka is included for comparison.

Figure 4-6 summarises the results obtained as described above, using, as an example, the statistics provided by /Bödvarsson et al. 2006/, i.e. for the frequency $f = 7.8\cdot10^{-8}$ year^{-1} per zone of earthquakes

Table 4-4. Cases of *occurrence* for a stability time of about 500,000 years.

End of Cycle 1	**End of Cycle 2**	**End of Cycle 3**	**End of Cycle 4**	**End of Cycle 5**	**End of Cycle 6**	**End of Cycle 7**	**End of Cycle 8**	**P2(10^6), per distribution**
120 ka	240 ka	360 ka	480 ka	600 ka	720 ka	840 ka	960 ka	
P1	🟩	🟩	🟩	**P1**	🟩	🟩	🟩	$P1^2$
P1	🟩	🟩	🟩	(1–P1)	**P1**	🟩	🟩	$(1-P1)\cdot P1^2$
P1	🟩	🟩	🟩	(1–P1)	(1–P1)	**P1**	🟩	$(1-P1)^2\cdot P1^2$
P1	🟩	🟩	🟩	(1–P1)	(1–P1)	(1–P1)	**P1**	$(1-P1)^3\cdot P1^2$
(1–P1)	**P1**	🟩	🟩	🟩	**P1**	🟩	🟩	$(1-P1)\cdot P1^2$
(1–P1)	**P1**	🟩	🟩	🟩	(1–P1)	**P1**	🟩	$(1-P1)^2\cdot P1^2$
(1–P1)	**P1**	🟩	🟩	🟩	(1–P1)	(1–P1)	**P1**	$(1-P1)^3\cdot P1^2$
(1–P1)	(1–P1)	**P1**	🟩	🟩	🟩	**P1**	🟩	$(1-P1)^2\cdot P1^2$
(1–P1)	(1–P1)	**P1**	🟩	🟩	🟩	(1–P1)	**P1**	$(1-P1)^3\cdot P1^2$
(1–P1)	(1–P1)	(1–P1)	**P1**	🟩	🟩	🟩	**P1**	$(1-P1)^3\cdot P1^2$

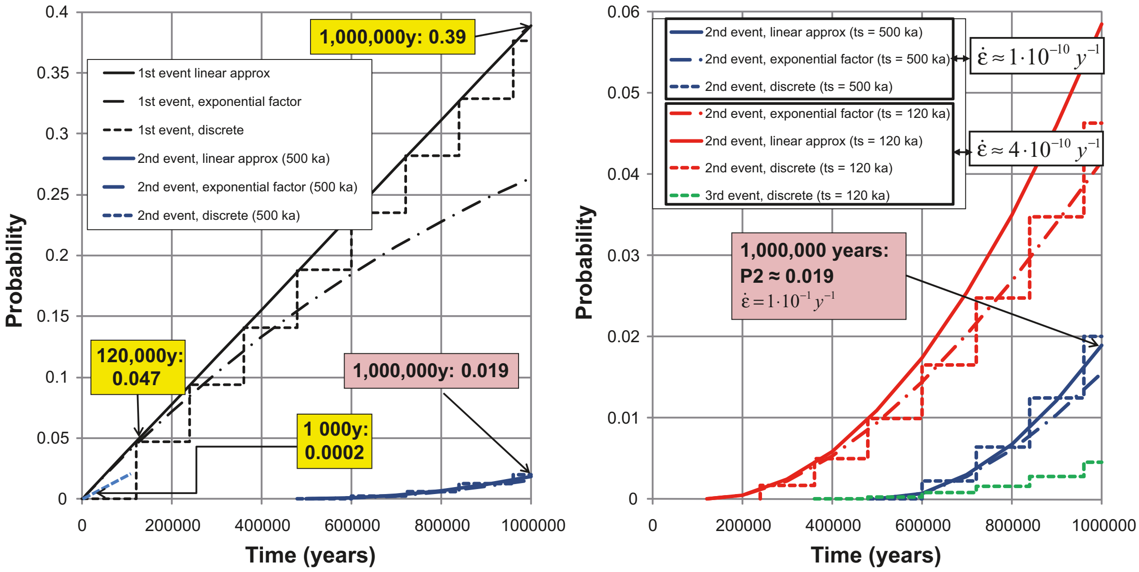

Figure 4-6. *Left: Probabilities used in SR-Site. Right: Sensitivity of probabilities of a second earthquake to the duration t_s of the period of local stability following a large strain energy release. Results for two values of t_s are shown; 120 ka and 500 ka. Corresponding strain rates are $4\cdot10^{-10}\cdot y^{-1}$ and $1\cdot10^{-10}\cdot y^{-1}$, respectively.*

of magnitude 5 or larger. Results are provided for different ways of approximating the probability evolution: using Equation 4-1, Equation 4-2 or the discrete step approach for P1, and Equation 4-4, Equation 4-5 or the discrete step approach for P2. Estimates in yellow boxes indicate the probabilities established as relevant for use in SR-Site (assessment of the number of canisters sheared 0.05 m or more) of one earthquake. The 1,000-year probability is set at a value that is intermediate to the probabilities obtained using the linear approximation (Equation 4-1) and the discrete step relation which allows for large earthquakes only during periods of endglacial instability. The estimate in the pink box shows the probability of a second earthquake established as relevant for use in SR-Site. The right part of the figure shows the sensitivity to the time required to restore stresses after a large earthquake. Assuming the time to be short enough for a large earthquake to occur at Forsmark at the end of all glacial cycles (i.e. every 120 ka) gives a modest increase of the probability of a second large earthquake within the 1 million year assessment period; a factor between two and three. For this to be a real possibility, the strain rate effective for restoring the stresses between glacial cycles would have to be $\dot{\varepsilon} = 4\cdot10^{-10}\cdot y^{-1}$, i.e. almost on par with the highest strain rates suggested for the large-scale tectonic compression of the Fennoscandian Shield. This would mean that there would be almost no aseismic strain energy release in large regional deformation zones at any time.

Therefore the value 0.019 suggested here for $P2(10^6)$ based on a lower strain rate ($\dot{\varepsilon} = 4\cdot10^{-10}\cdot y^{-1}$) is judged to be a relevant estimate.

If the stability time t_s does not cover three cycles (as the case shown in Table 4-4), there will be a non-zero probability $P3(10^6)$ of a third large earthquake within the one million year assessment time frame. The green discrete step relation in Figure 4-6 (right) shows the probability P3(t) for the worst case; unstable conditions at the end of all future glaciations, i.e. $t_s = 120{,}000$ years which requires a strain rate $\dot{\varepsilon} \geq 4\cdot10^{-10}\ y^{-1}$. At the end of the 1 million assessment period, the worst case probability P3 is less than 0.005.

Because of the low probability and the high strain rates required for a third earthquake, the possibility of a third large earthquake is not considered in SR-Site, i.e. in the assessment of the number of canisters sheared 0.05 m or more during the one million year assessment time frame. Additional reasons for not considering the possibility of more than two large earthquakes are listed below.

- The effects on the buffer-canister system of three (or more) small low-velocity slip events distributed over hundreds of thousands of years will be very different from those of one fast displacement that takes place in one single pulse of movement. Note that slip velocity scales with slip magnitude /Fälth et al. 2010/, meaning that the slip velocity effective for a displacement resulting from a number of smaller slip events is much lower than the reference slip velocity assumed in the stress-deformation analyses of the buffer-canister system performed to establish the damage threshold /Hernelind 2006/.

- The number of critical canisters will grow because accumulated slip will increase on small fractures. There are, however, limits to how much a small fracture can move without energy being spent on inelastic crack propagation at the fracture tips. Expending energy on crack propagation will limit the energy available for slip (cf. /La Pointe et al. 2000/.

The numbers given for the probabilities in Figure 4-6 as examples are based on frequency estimates given in /Bödvarsson et al. 2006/. Corresponding numbers are easily derived for other frequency estimates. Other approaches than the simplest possible (i.e. using Equation 4-1 for P1 and Equation 4-4 for P2) appear to give very similar results. The handling of the process "reactivation – displacements along existing discontinuities" is shown Figure 4-7. The various steps needed to assess the impact of one earthquake are indicated in the column of yellow boxes. The steps taken to assess the impact of the second earthquake are indicated in the column of pink boxes.

Model; Numerical procedure described in /Munier 2010/ for determination of the number of critical canisters.

Handling of variables influencing the process; The fracture geometry is included in the model.

Handling of variables influenced by the process; None of the variables are included in the model.

4.3.8 Uncertainties

Uncertainties in mechanistic understanding

Material models and fracture property data used in numerical models are usually derived from results of laboratory-scale shear box tests, in which samples are sheared tens of millimetres. For

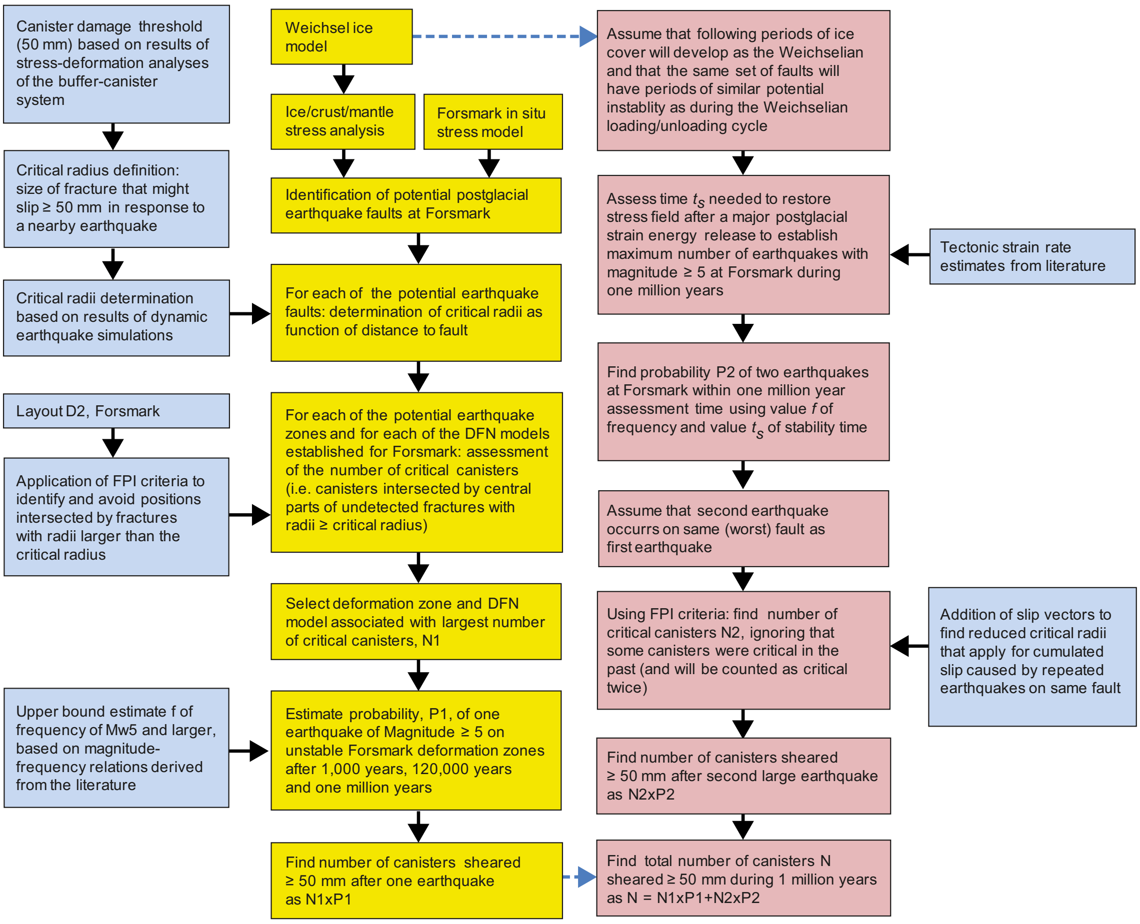

Figure 4-7. *Schematics of handling of fracture shear displacements generated by earthquakes.*

fractures in the rock mass, shear displacements depend upon the size of the fracture and the properties of the surrounding rock, meaning that large displacements can occur only on large fractures. A 5 mm displacement, for instance, would require a fracture radius of tens of metres, cf. Figure 4-3. It is uncertain how applicable any material model would be for the entire area of such large fractures.

Otherwise, there are no major uncertainties in mechanistic understanding for single fractures. For fracture zones, and, in particular, for large fracture zones, there is some uncertainty regarding their mechanical behaviour and their role in the development of the present-day stress fields. There is also some uncertainty regarding the conditions that determine whether displacements take place continuously or suddenly.

Model simplification uncertainties in SR-Site

There is an uncertainty regarding how the topography of the individual discontinuity on different scales influences its mechanical properties. Models for scale dependence exist, but no results from large-scale tests with non-planar fractures in constrained rock. The method that is applied in all the numerical modelling work described above, i.e. to regard all individual discontinuities as perfectly planar and with average properties uniformly distributed over the plane of the discontinuity, is pessimistic because non-planar fractures are likely to slip less. This relates to the point made above regarding uncertainties in mechanistic understanding.

Earthquakes: Except for the effect of a small number of explicitly modelled fractures, the host rock was assumed to be linear elastic in the dynamic 3DEC analyses described in /Fälth et al. 2010/, i.e. the calculated secondary displacements were not influenced by frictional or viscous damping. This may mean that secondary displacements were overestimated. The representation of the rupture in the earthquake simulations is very simplified and does not consider any variations of fault properties, for instance the fault residual strength /Fälth et al. 2010/. Instead the fault strength is ramped down to zero at all points on the rupture area without being affected by local and strong in-plane asperities. For a given stress field this will tend to overestimate the fault slip and the moment magnitude.

Input data and data uncertainties in SR-Site

For the excavation/operation period, the temperate period and the glaciation cycle, the handling is based on results obtained from models with generic fracture systems and with values of rock mass properties and fracture properties obtained from the site descriptive models. These data are set out in the SR-Site Data report /SKB 2010b/.

Earthquakes: The input data to the dynamic analyses used to derive the critical threshold radius are generic values of rock elasticity parameters and upper bound estimates of the stress drop for intraplate events.

The modulus of elasticity was set at 75 GPa, whereas the value for the two fracture domains containing the deposition areas at Forsmark is 69 and 70 GPa, respectively /Glamheden et al. 2007/. Overestimating the E-modulus will tend to underestimate the slip on target fractures for a given stress impact, but also to overestimate that stress impact, i.e. the stress redistribution and the amplitude of the stress waves generated by the slipping fault. Therefore, the net effects of small over- or under-estimates of the rock mass E-modulus are judged to be unimportant.

4.3.9 Adequacy of references supporting the handling in SR-Site

The supporting references /Bödvarsson et al. 2006/, /Lund et al. 2009/, /Hökmark et al. 2010/, /Lönnqvist and Hökmark 2010/, /Fälth et al. 2010/ and /Munier 2010/ are SKB reports that have undergone a documented factual- and quality review.

4.4 Fracturing

4.4.1 Overview/general description

When specimens of intact rock are loaded gradually in compression, i.e. subjected to increasing stresses, the initial deformations are elastic, but as the load increases a maximum stress is reached where the deformations become plastic or brittle. This maximum stress is the strength of the specimen under the given loading conditions. After further deformation, the specimen will fracture and its remaining load bearing capacity, its residual strength, is dependent solely on friction between the fragments.

The fundamental mechanism in the process, the growth of microfractures, was described by /Griffith 1924/. The application of Griffith's original fracture theory presupposes the existence of arbitrarily oriented elliptical cavities in a continuous elastic medium. The theory concludes that the uniaxial compressive strength is eight times that of the tensile strength, whereas the corresponding ratio for crystalline rocks is between 15 and 20. It has long been recognised that the Griffith Criterion was a crack initiation criterion that had little to do with crack propagation and hence with the peak strength of a brittle rock. Today, the most widely used failure criterion for describing the strength of intact rock and rock masses is the empirical failure model of Hoek-Brown /Hoek and Brown 1980/.

The fracturing process is dependent on the state of stress, and starts at lower loads than the failure load recorded in the uniaxial test under monotonic loading conditions. /Bieniawski 1967/ demonstrated that the development of the macro-scale fracture surface begins at approximately 80% of the failure load in uniaxial tests and /Lockner et al. 1992/ demonstrated that the same was also observed in triaxial compression tests. The phenomenon can be observed when tunnels and other cavities are excavated in rock at great depth where the primary stresses give rise to large stress concentrations. Next to the cavity walls, the tangential stresses are large and the radial constraint small, which can cause fracturing parallel to the cavity wall (spalling). For the walls of repository openings, the spalling strength may be as low as 40% of the uniaxial compressive strength /Martin et al. 2001/. In the APSE experiment, the spalling strength of Äspö Diorite was concluded to be 56% of the uniaxial strength /Andersson 2005/. /Martin 1997/ proposed that this difference between *in situ* strength and laboratory strength was due to the loading path, i.e. the loading path *in situ* is far more complex than the loading path in uniaxial and triaxial laboratory tests.

The mechanisms that control the growth of microfractures in principle also control the propagation of existing fractures. In confined rock, an individual fracture can propagate by growing in its own plane by means of shear failure (sliding crack), and by fracturing at an angle to its own plane by tensile failure at the periphery of the fracture, so-called "splay cracks" or "wing cracks" /Scholz 1990/.

Hydraulic fracturing may occur if the effective normal stress across a fracture reaches the tensile strength. This is a theoretically possible effect of significantly increased pore pressures combined with modest increases in mechanical stresses, for instance during a glacial cycle /Hökmark et al. 2006/.

4.4.2 Dependencies between process and geosphere variables

Table 4-5 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 4.4.7.

Table 4-5. Direct dependencies between the process "Fracturing" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	**Variable influence on process**			**Process influence on variable**		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Temperature in bedrock	No. But indirectly via thermal stress.	–	See Section 4.2.	No.	–	–
Groundwater flow	No.	–	–	No. But indirectly through changes in fracture geometry.	–	–
Groundwater pressure	Yes. Hydraulic fracturing at high pressures.	All	Included in the model as fracture pore pressure.	No.	–	–
Gas phase flow	No.	–	–	No. But indirectly through changes in fracture geometry.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Repository geometry	No. But indirectly through stresses.	–	–	No.	–	–
Fracture geometry	No. But indirectly through stresses.	All	See Section 4.3.	Yes. But changes will be modest compared with existing fractures.	Excavation/ operation	Scope and extent of fracturing in near-field rock evaluated from stress results and observations from the APSE experiment. Handling of EDZ effects based on schematic assignment of transmissivity value to fictitious tunnel floor fracture.
					Temperate	Scope and extent of fracturing in near-field rock evaluated from stress results and observations from the APSE experiment.
					Periglacial	Risk of hydraulic fracturing evaluated from stress results.
					Glacial	Evaluated from stress results, including risk of hydraulic fracturing.
Rock stresses	Yes.	Excavation/ operation	Site-specific rock stresses.	Yes.	All	No handling. Output from model shows that stress relaxation effects of fracturing are limited to small volumes.
		Temperate	Thermal stresses calculated in model.			
		Periglacial	Stresses calculated in model			
		Glacial	Stresses at repository depth from ice/crust/ mantle model, /Lund et al. 2009/. Otherwise same as for temperate period.			
Matrix minerals	Yes. Affects rock strength.	All	Site-specific rock mechanics property data.	No.	–	–
Fracture minerals	Yes. Strength of individual fractures depends on fracture minerals and will contribute to determine extent of fracture growth.		Neglected. Covered by strength ranges applied in fracturing assessment.	Yes. Fracturing can create new fracture surfaces with different mineralogy.	All	Not considered in SR-Site. New fractures will contribute an insignificant portion of the total fracture area.
Groundwater composition	No.	–	–	No. But indirectly by the creation of new fracture surfaces.	–	–
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	Yes. Affects strength properties.	All	Neglected; effect is negligibly small.	No.	–	–

Temperature in bedrock; There are no indications that the temperature dependence of strength of intact rock is such that fracturing or fracture propagation could be impeded or promoted, at least sufficiently to need to be considered in the safety assessment. The energy expended on fracturing is too minor to have any influence on the temperature. In the walls of deposition holes, tangential thermal stresses will be high and are likely to cause spalling in cases where slow water supply delays the development of a supporting bentonite swelling pressure.

Groundwater flow; Groundwater flow variations will not promote or impede fracturing. Fracturing will cause some permeability increase, which will affect the groundwater flow. The formation of an EDZ around tunnels during construction is the most important aspect of this.

Groundwater pressure; Large pressures may cause hydraulic fracturing. Fracturing cannot have any effect on the groundwater pressure.

Gas phase flow; There will be no mechanical effects of gas flow variations. Similar to groundwater flow, there will be changes in the gas flow conditions when fractures are formed or propagate.

Repository geometry; The geometry (location of individual fractures relative to openings, tunnel orientation relative to *in situ* stress field, tunnel shape and canister spacing) will influence the stress state and affect the scope and extent of fracturing around the repository openings. Fracturing cannot change the repository geometry.

Fracture geometry; The fracture geometry is important to the process: fracture propagation takes place at the tips of existing fractures. Intact rock failure is promoted in regions where slipping fractures create stress concentrations. By definition, fracturing will change the geometry of the fracture system. However, compared with the size and frequency of existing fractures, these changes will be modest.

Rock stresses; The stress state has a decisive impact on the scope and extent of fracturing. When fracturing takes place because of stress concentrations, for instance at the periphery of tunnels and deposition holes, the effect of the fracturing will be to relax and redistribute some of the stresses. Fracturing caused by, for instance, blasting will affect the stresses in a similar way.

Matrix minerals; The composition of matrix minerals in different rock types determines their mechanical properties, for instance the strength properties which are important to fracturing. Fracturing cannot affect the composition of matrix minerals.

Fracture minerals; Fracture minerals contribute to determine the strength of individual fractures and the conditions controlling fracture growth. Fracturing can expose new fracture surfaces with different mineralogy.

Saturation; Differences in strength properties between saturated and unsaturated samples of rock may exist, cf. e.g. /Jacobsson and Bäckström 2005/. Dry samples tend to have a higher strength. The differences are, however, small and pessimistically neglected. All strength estimates in SR-Site are based on results of tests performed on wet samples, cf. /Glamheden et al. 2007/.

4.4.3 Boundary conditions

The peripheries of the repository openings and the ground surface are the boundaries of the geosphere for all mechanical processes. Mechanically, these boundaries are subject to the same type of boundary condition throughout the entire repository lifetime, i.e. a state of more or less well-defined normal and shear stresses. At the opening peripheries, the boundary stress will be zero before deposition and backfilling. Some time after closure the boundary stress will correspond to the swelling pressure of the bentonite buffer for deposition holes and to the swelling pressure of the backfill for deposition tunnels. When the pore pressure increases in the near field as a result of the restoration of the groundwater pressure, there will be a corresponding increase of the boundary stress at the walls of the openings. The ground surface will be at zero normal stress at all times except for the glaciation period, when the normal boundary stress will vary according to the ice-model assumed to apply.

4.4.4 Model studies/experimental studies

The progressive failure of intact rock has been studied by many researchers, e.g. /Martin and Chandler 1994/ and /Li 1993/. In the initial elastic phase, the specimen's existing microfractures are first compressed. Then a stable growth of extensional microfractures occurs in the direction of the largest principal stress. Before failure occurs, i.e. before the limit of the strength of the specimen has been reached, a phase takes place with unstable growth of the microfractures, either as before in the direction of the largest principal stress, or where macro-scale shear fractures form by the interaction and coalescing of microfractures. The way in which fracture growth occurs is dependent on the rock properties and the load. Under uniaxial load, the unstable growth and the macroscopic fracturing occur axially, i.e. in the direction of the largest principal stress. In constrained specimens, macroscopic shear fractures can form.

Whether an existing fracture propagates, and in what direction this propagation occurs, depends on the local stress field at the fracture periphery /Scholz 1990/. Numerical models for prediction of propagation in elastic media, based on application of strain energy criteria, have been tested in 2-dimensional, near-field analyses /Shen and Stephansson 1996/. The results showed that the process presupposes high stress levels and strong stress anisotropy. If the ratio between the largest and smallest primary principal stress was greater than 4, propagation and coalescence of individual fractures around circular cavities occurred.

/Fälth and Hökmark 2007/ performed thermomechanical elastic 3D calculations of the state of stress around deposition holes. Rock in a potential failure state after heating was found only in small volumes along the most stressed parts of the borehole peripheries. The maximum depth of potential failure from the wall of the deposition hole was about 150 mm.

At the 420 m level in the URL in Canada, brittle failures with rock breakout were obtained along nearly vertical lines in two vertical 600 mm holes bored in the floor of a tunnel in fracture-poor rock with large primary stresses. However, no failure was obtained in the uppermost part of the holes, on a level with the tunnel's EDZ. In a subsequent heating phase with peak temperatures of between 80 and 90°C at the borehole walls, the failure-zone extended to become continuous all the way down to the borehole bottoms. However, no failure was recorded in the tunnel's EDZ /Martino and Read 1995/. The depth of the brittle failures was about 50 mm, measured from the borehole walls.

The APSE experiment /Andersson 2003, 2005/ specifically addressed the problem of spalling in the walls of deposition holes. A tunnel with a rounded floor was excavated by use of a careful blasting technique in sparsely fractured rock. The tunnel axis was perpendicular to the major stress. The rounded floor, the tunnel orientation and the excavation technique together gave high tangential stresses in the floor region. A deposition hole was drilled in the centre of the highly stressed floor and then pressurised by use of a water-filled bladder. A second hole was drilled at 1.0 m distance from the first one along the line of the tunnel axis. Vertical rod-shaped heaters were installed close to the side of the slender, now highly stressed, pillar. The tangential stress in the pillar could be further increased by reducing the support pressure in the bladder and by increasing the heat load. In the second hole, spalling occurred as response to excavation, heating and bladder pressure reduction. Each of these measures taken to increase the tangential stress extended the breakout zone some decimetres further down the hole. Back-calculations indicated that spalling in the second hole occurred at a tangential stress corresponding to about 57% of the uniaxial compressive strength. The geometry of the failed zone was similar to that found in the URL test described above. Recordings of acoustic emission data as well as the visual inspection of the rock walls during the experiment supported the hypothesis that very small confining pressures are sufficient to suppress initiation and propagation of brittle failures.

The CAPS experiment was carried out by /Glamheden et al. 2010/ particularly to find out if the small support pressure provided by a loose filling of bentonite pellets in the annular space between bentonite blocks and rock wall would be sufficient to prevent thermally-induced spalling in KBS-3 deposition holes. Eight 4 m-deep, 0.5 diameter holes were drilled in the tunnel previously used for the APSE experiment. The holes were heated by central heaters; four holes were left open and four holes had a supporting pellets filling. In the open holes, spalling occurred largely as expected, i.e. at a level of stress corresponding to about 57% of the uniaxial compressive strength. Because of rock inhomogeneities and differences in relative humidity, however, spalling appeared to occur sporadically in some of the holes and more systematically in others. After noting that the results were highly variable and not totally consistent, presumably because of different saturation conditions and the rock inhomogeneity, /Glamheden et al. 2010/ nevertheless concluded that the support pressure provided by the loosely filled pellets limited the growth and extension of the spalled zone very efficiently, even if it did not completely inhibit crack formation. Injection tests performed in the supported, potentially fractured, part of the wall indicated that no continuous zone of increased permeability had formed.

4.4.5 Natural analogues/observations in nature

Not applicable.

4.4.6 Time perspective

See Section 4.3 "Reactivation – displacement along existing fractures".

4.4.7 Handling in the safety assessment SR-Site

Excavation/operation period

Estimates of the scope and extent of fracturing, e.g. spalling in deposition holes, are made using results obtained from 3DEC near-field models, and by use of observations from the isothermal phase of the APSE experiment. The effects of fracturing around deposition tunnels caused by drilling and blasting, i.e. the effects of an EDZ, is estimated to correspond to the effects of a $1\cdot10^{-8}$ m^2/s fracture below the tunnel floor, cf. the SR-Site Data Report /SKB 2010b/.

Model; The 3DEC model described in /Hökmark et al. 2010/.

Boundary conditions; Zero normal and shear stress assigned to all boundaries (see general boundary condition statement above).

Handling of variables influencing the process; Rock stresses are included in the model. Statements on the influence of groundwater pressure and fracture geometry are made based on the findings made in the modelling performed for the SR-Can assessment /Hökmark et al. 2006/. Mineral composition determines the values of property parameters and is included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model. There is, however, no handling of stresses in volumes of failed (spalled) rock.

In a general context, excavation activities may induce violent seismic fracturing events. Data from deep South African mines show that rocks in an environment with non-existing faults and with low fracture densities and high stresses might generate faults in a previously unfractured rock mass /Bäckblom and Munier 2002/. Seismic events other than slip along existing faults have magnitudes that are typically less than 3.5 and require *in situ* stresses above 50% of the unconfined intact rock strength /Martin et al. 2001/. To produce seismic events more severe than minor slabbing, the major *in situ* stress must be about 40% of the unconfined compressive intact rock strength, i.e. typically 70–85 MPa.

The repository will be located in fractured bedrock at intermediate depth where the maximum stresses are not more than about 25% of the unconfined strength. In addition, the extraction ratio will be much smaller than in mines, where seismic events are known to have been triggered by excavation activities. Therefore, the possibility of excavation-induced seismicity is not considered in SR-Site.

Temperate climate domain

Estimates of the scope and extent of fracturing, e.g. thermally induced spalling in unsupported and dry deposition holes, are made by use of modelling results obtained from 3DEC near-field models and by use of observations from the heated phase of the APSE experiment /Andersson 2005/.

Model; The 3DEC model described in /Hökmark et al. 2010/.

Boundary conditions; Zero normal and shear stress assigned to the ground surface and at the walls of the repository openings.

Handling of variables influencing the process; Rock stresses are included in the model. Statements on the influence of groundwater pressure and fracture geometry are made based on the findings in the modelling performed for the SR-Can assessment /Hökmark et al. 2006/. Mineral composition determines the values of property parameters and is included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model. There is, however, no particular handling of stresses in volumes of failed (spalled) rock. There is no particular handling of the effects on gas flow, since the main concern regarding gas and gas generation is the possibility of gas being trapped in the buffer and at the rock/buffer interface (cf. gas flow/dissolution process, Section 3.2).

Periglacial climate domain

During periglacial conditions, the state of stress in the near field is determined by background stresses that are approximately the same as the present-day undisturbed *in situ* stresses, whereas the buffer and the backfill will have reached full saturation and, consequently, will stabilise the peripheries and suppress fracturing. Even the worst case climate assumptions do not give frozen ground depths in excess of 422 m or freezing of buffer or backfill /SKB 2010d/and, consequently, no effects of ice formation in fractures. This means that there is no potential for fracturing in excess of that already accounted for in the previous sections (excavation/operation and temperate periods) and that no modelling of fracturing in the near-field is required. The risk for hydraulic fracturing because of high pore pressures is assessed in /Lönnqvist and Hökmark 2010/.

Glacial climate domain

Estimates of the scope and extent of fracturing in the near field are made using results obtained from 3DEC near-field models. The risk of hydraulic fracturing because of high pore pressures is assessed in /Lönnqvist and Hökmark 2010/.

Model; The 3DEC model described in /Hökmark et al. 2010/ (near field). Analytical method described in /Lönnqvist and Hökmark 2010/ (hydraulic jacking).

Boundary conditions; Normal stress assigned at the ground surface, horizontal stress at repository depth according to ice/crust/mantle model /Lund et al. 2009/ and zero pressure on walls of openings (near field). Liquid pressure corresponding to overburden stress at ground surface (hydraulic jacking).

Handling of variables influencing the process; Groundwater pressure, fracture geometry and rock stresses are included in the model. In addition, the scope and extent of pore pressure-induced hydraulic fracturing is estimated. Mineral composition determines the values of property parameters and is included indirectly.

Handling of variables influenced by the process; Stresses are calculated in the model.

Earthquakes

Fracturing directly associated with earthquake faulting is included in the rupture propagation model used in the earthquake simulations without detailing the nature of the process. Case studies of earthquake-induced damage to underground facilities show that fracturing is confined to the immediate vicinity of the earthquake fault /Bäckblom and Munier 2002/. This holds true for open tunnels at much shallower depths than that of the repository. Around backfilled tunnels at 500 m depth, fracturing will be even less significant. Therefore the process is ignored.

4.4.8 Uncertainties

Uncertainties in mechanistic understanding

The principles of the process are mostly well understood. The mechanisms by which the stress path influences the strength in the walls of deposition holes such that spalling occurs at stress levels below the laboratory-determined failure load are not fully understood. There is also an uncertainty as to whether microcracking could induce creep and subsequent failure at lower stress levels than the spalling strength. However, to model the process well enough to reproduce the shape, size and location of failed regions around repository openings requires extensive calibration work with discontinuum modelling tools, such as the PFC code /Martin et al. 2001/. For the above handling in SR-Site, an understanding of the nuances of the process is not essential.

Model simplification uncertainties in SR-Site

The hydraulic properties of the EDZ are not assessed by means of numerical modelling. The EDZ hydraulic models are based on empirical findings from tunnelling with careful drill and blast methods.

The numerical analyses described above, which are used to assess the scope and extent of fracturing around deposition holes, do not include modelling of the fracturing process. Simple, linear elastic models are analysed to find the stress levels and to determine the size of the volumes in which the spalling strength may be reached.

The codes for modelling of fracture propagation that have been tested are 2-dimensional, which presumably means that the extent of the process is overestimated, i.e. that individual fractures propagate more than they would in a 3-dimensional model with varying conditions along the fracture perimeter. It is also uncertain what potential for large displacements a fracture created by fusion of two imperfect coplanar fractures may have. The fracture extension that sets the limit for the possible displacement along such a fracture can reasonably be assumed to be less than the sum of the extensions of the two original fractures.

Input data and data uncertainties in SR-Site

For the excavation/operation period, the temperate period and the glacial episode, the handling is based on results obtained from models with generic fracture systems and with values of rock mass properties and fracture properties obtained from the site descriptive models. The input, including the uncertainties specified in the site descriptive models, is reported in the SR-Site Data report /SKB 2010b/. Empirical data are obtained from the APSE experiment. These data are also given in the SR-Site Data report /SKB 2010b/.

4.4.9 Adequacy of references supporting the handling in SR-Site

The supporting references /Glamheden et al. 2010/, /Lund et al. 2009/, /Hökmark et al. 2010/, /Lönnqvist and Hökmark 2010/ and /Munier 2010/ are all SKB reports that have undergone a documented factual and quality review.

4.5 Creep

4.5.1 Overview/general description

The concept of creep implies that a material has inherent time-dependent mechanical properties, so that displacements take place due to already active stresses without additional loading.

In laboratory-scale constant load tests of intact rock samples, the creep strain rate can be recorded as a function of time for different loading conditions. For crystalline rock samples, the process is controlled by time-dependent microcrack growth. Such experiments show that creep rates decay fast unless the load exceeds a significant fraction, between 1/3 and 2/3, of the failure stress /Pusch and Hökmark 1992/. Extrapolating strain rates that have been recorded during constant load tests suggests accumulated total strains of between 0.1% and 0.3% after about 1 million years /Glamheden and Hökmark 2010/, meaning that creep in intact rock is not a concern for the deep repository. This statement is supported by conclusions drawn by /Damjanac and Fairhurst 2010/ regarding long-term strength thresholds in crystalline rock. Damjanac and Fairhurst establish that "stress corrosion", which is the generally accepted mechanism for time-dependent weakening of crystalline rocks, is a process by which chemical environmental effects reduce the surface energy of induced cracks (i.e. the fracture toughness) and thereby allow fracture growth. Stress corrosion reactions are likely to be among the mechanisms giving "subcritical crack growth" /Potyondy 2007/. The process requires the existence of cracks with tensile conditions at the crack tips, meaning that confinement will suppress fracture growth by stress corrosion. Results of a numerical analysis by /Damjanac and Fairhurst 2010/ indicated that confinement corresponding to less than 2% of the compressive load would be sufficient to stabilise a sample of crystalline rock loaded to 56% of the short-term strength, even if stress corrosion had reduced the strength to zero. More generally /Damjanac and Fairhurst 2010/ conclude that a "stress threshold" (i.e. a deviatoric stress that can be sustained indefinitely) exists for crystalline rocks. The threshold is likely to be about 40–60% of the compressive strength. Conditions for creep in intact repository rock are therefore likely to be found only in the most stressed parts of the deposition hole walls, i.e. where the potential impacts of creep are covered by the assumptions made regarding spalling (cf. Section 4.4)

In jointed rock masses of crystalline rock, all significant creep can be approximated to occur along fractures and fracture zones /Glamheden and Hökmark 2010/.

The driving force behind creep displacements is the occurrence of deviatoric stresses. Theoretically, rock mass creep deformations (i.e. shear displacements along fractures and fracture zones) may proceed either until no deviatoric stresses remain, or until the deviatoric stresses have been sufficiently reduced. The mechanisms controlling the creep process in fractures are described in /Pusch and Hökmark 1992/ and /Glamheden and Hökmark 2010/. For unfilled fractures, the properties of the fracture surfaces are important to the process. It depends, for instance, on the strength and geometry of successively damaged interlocking asperities. For filled fractures, the filling thickness and the type of filling material contribute to control the process. Findings in the literature on creep displacements along fractures suggest that significant creep in fractures will not occur unless the shear stress magnitude is above some threshold value /Amadei and Curran 1982, Bowden and Curran 1984, Schwartz and Kolluru 1982/. The threshold stress may roughly be estimated to be about 30% of the nominal fracture shear strength for unfilled fractures and to be about 10% for filled fractures /Glamheden and Hökmark 2010/. The long term strength of fractures and fracture zones at Forsmark, however, seems to be sufficient that the rock mass has sustained significant deviatoric stresses for very long periods of time. Therefore, for the Forsmark fractures, creep displacements are likely to be insignificant compared to displacements caused by the direct changes in load and pore pressure projected for the different phases of the assessment period.

4.5.2 Dependencies between process and geosphere variables

Table 4-6 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 4.5.7.

Table 4-6. Direct dependencies between the process "Creep" and the defined geosphere variables and a short note on handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes.	All	Process neglected. Effects covered by processes 4.3 and 4.4.	No.	–	–
Groundwater flow	No.	–	–	No. But indirectly through changes in fracture geometry.	–	–
Groundwater pressure	Yes. Affects fracture strength.	All	Process neglected. Effects covered by processes 4.3 and 4.4.	No.	–	–
Gas phase flow	No.	–	–	No. But indirectly through changes in fracture geometry	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Repository geometry	No. But indirectly through stresses.	–	–	No.	–	–
Fracture geometry	Yes.	All	Process neglected. Effects covered by processes 4.3 and 4.4.	Yes.	All	Process neglected; effect is small and cannot be separated from direct effects of stress changes.
Rock stresses	Yes. Deviatoric stress state is necessary for the process.	All	Process neglected. Effects covered by processes 4.3 and 4.4.	Yes.	All	Process neglected.
Matrix minerals	Yes. Strength of asperities has impact on fracture properties.	All	Process neglected. Effects covered by processes 4.3 and 4.4.	No.	–	–
Fracture minerals	Yes. Mineral-filled fractures will probably exhibit more creep than clean fractures.	All	Process neglected. Effects covered by processes 4.3 and 4.4.	No.	–	–
Groundwater composition	No. But indirectly via properties of fracture filling materials affected by changes in groundwater composition.	–	–	No.	–	–
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	No.	–	–	No.	–	–

Temperature in bedrock; Creep displacements may be promoted by high temperatures. For the bounding type estimates made in SR-Site, this is not important.

Groundwater flow; The groundwater flow may move fracture material and change fracture properties and indirectly affect creep. Creep displacements may change apertures and transmissivities of fractures.

Groundwater pressure; High groundwater pressures will reduce the shear strength of fractures and promote creep. The impact of the groundwater pressure on the process is similar to its impact on the reactivation process.

Repository geometry; The repository geometry influences the stresses, but there are no direct couplings to the process.

Fracture geometry; The process is mainly slow displacements along fractures and is therefore determined by the fracture geometry. Creep deformations can change the fracture geometry, for instance because of fracture growth in unconfined rock, but the effects are small and cannot be separated from direct effects of stress changes.

Rock stresses; Creep deformations are driven by and relax deviatoric stresses. Extensive creep deformations will tend to transform anisotropic stress states into more isotropic ones. In stable shield regions, however, stress relaxation because of creep does not seem to be important: In Forsmark, high deviatoric stresses are measured at all depths considered in the site investigation.

Matrix minerals; The matrix mineral composition contributes to determine the mechanical properties of fracture surfaces, e.g. strength of asperities.

Fracture minerals; Mineral-filled fractures will probably exhibit more creep than clean fractures. The process is not known to have any influence on the composition or abundance of fracture minerals.

4.5.3 Boundary conditions

The peripheries of the repository openings and the ground surface are the boundaries of the geosphere for all mechanical processes. Mechanically, these boundaries are subject to the same type of boundary condition throughout the entire repository lifetime, i.e. a state of more or less well-defined normal and shear stresses. At the opening peripheries, the normal and shear boundary stresses will both be zero before deposition and backfilling. Some time after closure the normal boundary stress will correspond to the swelling pressure of the bentonite buffer for deposition holes and to the swelling pressure of the backfill for deposition tunnels. The ground surface will be at zero normal stress at all times except for the glaciation period, when the boundary normal stress will vary according to the ice-model assumed to apply.

4.5.4 Model studies/experimental studies

The displacements in the dome in SFR, a repository for low- and intermediate level radioactive waste at Forsmark, have been measured with extensometers since the blasting was concluded in 1985 /Pusch 2003/. The measured displacements are unsystematic and so small in relation to the accuracy of the extensometers that interpretation, as well as prediction of possible continued displacement, is difficult. Furthermore, the dome is reinforced with bolts and shotcrete.

Results from plate loading tests on rock have shown that the creep strain rates at constant load typically decline logarithmically with time /Pusch and Hökmark 1992/.

A numerical model of a circular tunnel, in which the rock material nearest the tunnel periphery was assumed to have time-dependent deformation properties, gave a maximum radial creep displacement of 0.3 mm after approximately 2,000 years /Pusch and Hökmark 1992/. /Eloranta et al. 1992/ found that it would take about 10^9 years for the deposition hole wall to move 10 mm radially, provided that the rock around the deposition hole is of good quality. /Damjanac and Fairhurst 2010/ simulated fracture growth by stress corrosion in crystalline rock using a model for strength reduction at the tip of a growing fracture. Very modest confining pressures were found to suppress the process and stabilise the rock, even after having reduced the strength to zero.

/Glamheden et al. 2004/ conducted calculations of creep convergence of KBS-3 deposition tunnels with 3DEC. Creep displacements were assumed to take place along discontinuities only. The time aspect of the creep processes was not explicitly included. Instead, the effects of creep (i.e. successive relaxation of shear stresses on fractures) were replicated by allowing fractures to move using a scheme for successive fracture shear strength reduction. The reduction scheme was based on the notion of creep thresholds derived from a literature study on creep along discontinuities /Glamheden and Hökmark 2010/. The threshold stress was set at 30% of the nominal fracture shear strength. The results showed that creep could cause a tunnel wall displacement of about 2 cm for a fracture system with a high fracture frequency (2 m^2 of fracture area per m^3 of rock volume) of unfilled fractures with extensions of tens of metres. All fractures were parallel with the tunnel axis. Because of the high fracture density, the orientation of the fractures and the low creep threshold, the 2 cm displacement was concluded to be an upper bound estimate. /Hökmark 2003/ calculated displacements in the near field of a KBS-3 deposition hole with 3DEC, using a fracture geometry based on a statistical discrete fracture model established for the Äspö HRL prototype repository rock mass. The strength properties of the fractures were reduced in steps to about 40% of the initial strength, i.e. almost to the threshold value suggested in the general overview above. This relaxation of fracture shear stresses caused convergence of a deposition hole of less than 1 mm.

4.5.5 Natural analogues/observations in nature

Horizontal stresses, measured in unfractured rock at shallow depths in the stable Canadian Shield plate region, are of magnitudes that are consistent with a tectonic compression that has taken place over many millions of years /Damjanac and Fairhurst 2010/. This indicates that the rock has sustained high deviatoric stresses under unconfined conditions for very long periods of time and supports the notion that creep in crystalline rock material is not an issue for the safety assessment.

4.5.6 Time perspective

The process will by definition take place during all phases.

4.5.7 Handling in the safety assessment SR-Site

Excavation/operation period

The process is not considered. The creep displacements that take place during the operation phase do not need to be separated from the displacements that take place as a direct response to excavation.

Temperate climate domain

If it is assumed that all significant displacements take place along fractures, then the ultimate consequence of extensive creep displacements over a long period of time is that the fracture shear stresses eventually will decrease to zero. There is no evidence anywhere in the world where deep mining is carried out in hard rocks that such a condition exists, i.e. deviatoric stresses are recorded at all mine sites.

During the heated period of the temperate phase, gently dipping fractures and fractures located close to the excavated openings may be sheared because of the increased shear loads. If there is a thermally induced, time-dependent strength degradation of the fractures, some additional displacement could theoretically take place in the form of creep movement. However, apart from the nearest surroundings of the deposition holes, temperature increases are modest, 50 m above or below the repository horizon the temperature increase is not more than about 20 degrees. Between deposition areas the increase is about 10 degrees /Hökmark et al. 2010/. Therefore creep deformations, if any, are judged likely to be small. Additionally, the majority of the fractures will be stabilised rather than destabilised throughout the heated period, cf. /Hökmark et al. 2010/.

Intact rock creep requires stresses that will be found only in small volumes around the walls of the openings /Hökmark 2003/. The effects are accounted for in the assessment of thermally-induced spalling, cf. Section 4.4.

Because of the above, creep along fractures as well as creep in intact rock is neglected in the period of temperate conditions.

Periglacial and glacial climate domains

The process is neglected for the same reasons as for the temperate period. During the glaciation cycle, stresses will be higher /Hökmark et al. 2010, Lund et al. 2009/, but not sufficiently high to change the outcome of the estimates.

Earthquakes

Not applicable.

4.5.8 Uncertainties

Uncertainties in mechanistic understanding

The present day mechanistic understanding of creep in crystalline rock is adequately summarised in /Damjanac and Fairhurst 2010/. The uncertainties are judged to be small. For creep along fractures and fracture zones, the summary given by /Glamheden and Hökmark 2010/ is judged to be adequate. Here, however, the uncertainties are larger, mainly because there are few observations on relevant scales.

Model simplification uncertainties in SR-Site

The uncertainties associated with the simplification of the creep problem, i.e. to neglect creep altogether, are judged to be small. Creep in crystalline rock is a process that, if it occurs at an extent relevant for the repository, is not consistent with the anisotropic stress states found in stable shield areas.

Input data and data uncertainties in SR-Site

No data are used in SR-Site.

4.5.9 Adequacy of references supporting the handling in SR-Site

The references /Glamheden et al. 2010/, /Hökmark et al. 2010/ and /Hökmark et al. 2009/ are SKB reports that have undergone a documented factual and quality review. The reference /Damjanac and Fairhurst 2010/ is a peer-reviewed article that is available in the open literature.

4.6 Erosion/sedimentation in fractures

4.6.1 Overview/general description

In order to describe the erosion of materials in the fractures, two different systems have to be considered. First, the driving forces from the groundwater and secondly the resistant force expressed through the strength of the material in the fractures.

Groundwater

The erosive force is created by flowing groundwater. Stagnant groundwater does not affect the fracture filling by any mechanical force, but can affect the fillings by chemical reactions which are not considered here, but in Section 5.6. The groundwater flow is driven by a hydraulic gradient. This could either be natural groundwater flow that, in general, is driven by gradients in surface elevation but which can be emphasised by the passage of an ice front, or it could be caused by the effect of excavation in the rock which creates a local hydraulic gradient. This local gradient is in general magnitudes larger than that due to topography. As water flows, the friction in the fluid induces a drag at the fracture surfaces. This also means that a shear stress, which can be determined by studying the energy equations for a flowing medium, acts at the fracture surfaces. The shear stress may at high gradients act as an erosive force on the fracture fillings. This means that the largest gradients will apply during the construction, operation and early saturation phase, and hence the largest erosive forces from the groundwater will act over this period.

Fracture materials

The material in the fractures can be divided into fracture filling and gouge. The filling is here defined as material that is bonded to the surrounding rock whereas the gouge is loose material in the fractures.

The erosion of material can lead to a re-arrangement of the fracture filling/gouge by erosion and then sedimentation further down stream resulting in a re-arranged hydraulic conductivity of the zones. During the construction, operation and early saturation phase, there is also a possibility that fracture filling/gouge will be transported into the excavated areas and this could lead to an increased hydraulic conductivity in the eroded fractures. There is also a potential for erosion of bentonite, which means that bentonite would be transported along the groundwater flow direction and deposited in adjacent fractures.

In terms of gouge material, its general friability will facilitate removal and transport. The amount of gouge is highly dependent on the location and on the specific fracture zone considered. In Forsmark, for example, the amounts of gouge material are very limited /SKB 2008a/.

4.6.2 Dependencies between process and geosphere variables

Table 4-7 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 4.6.7.

Table 4-7. Direct dependencies between the process "Erosion/sedimentation in fractures" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	No.	–	–	No.	–	–
Groundwater flow	Yes.	All, but mainly during construction and glacial front passage	The process is neglected. Although the flow in large fractures at depth might be significant the shear force is still very low (see Section 4.6.7).	No. But, indirectly by rearrangement of material in the fractures changing the fracture geometry.	–	–
Groundwater pressure	Yes. This variable is strongly connected to flow.	All	Process neglected; see row Groundwater flow above.	No. See row Groundwater flow above.	–	–
Gas phase flow	Yes. But expected gas flow is too low to accomplish erosion.	All	Process neglected; No gas flow sufficiently strong is expected, see row Groundwater flow above.	No. But, indirectly by changing the fracture geometry.	–	–
Repository geometry	No. As long as the design aims at avoiding larger zones at great depths where erosion can be an issue.	–	–	No.	–	–
Fracture geometry	Yes.	All	Process neglected; see row Groundwater flow above.	Yes.	All	Process neglected; site observations indicating limited significance at repository depth.
Rock stresses	No.	–	–	No.	–	–
Matrix minerals	Yes. Bonding with fracture fillings depends on the matrix minerals.	All	Neglected since the bonding strength is much larger than the erosive force.	No.	–	–
Fracture minerals	Yes. They are potentially eroded away. Their nature will influence the process.	All	Process neglected; see row Groundwater flow above.	Yes.	All	Process neglected; see row Fracture geometry above.
Groundwater composition	Yes. Very diluted waters will favour the re-suspension (erosion) of colloidal-sized materials in fractures.	All	Process neglected; see row Groundwater flow above.	Yes. Mechanical erosion may increase the concentration of colloids. Indirectly the exposure of new mineral surfaces will induce reactions between groundwater and minerals.	All	Process neglected; see row Fracture geometry above.
Gas composition	No.	–	–	No.	–	–

Variable	Variable influence on process Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Process influence on variable Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Structural and stray materials	Yes. Grouting is potentially eroded away. Its nature will influence the process.	All	Process neglected; see row Groundwater flow above.	Yes. Redistribution through erosion-sedimentation.	All	Process neglected; see row Fracture geometry above.
Saturation	Yes.	All	Neglected; in unsaturated rock volumes the expected gas flow is too low to cause erosion.	No.	–	–

4.6.3 Boundary conditions

The most important geosphere boundary is the groundwater table which governs the groundwater pressure and hence is an important parameter for the hydraulic gradient.

4.6.4 Model studies/experimental studies

The studies performed on the force from the groundwater and the strength of the fracture filling/gouge are presented separately. In order to describe the potential for erosion, these findings are then compared.

Groundwater

In /Axelsson 2006/, the governing equations for erosion of fresh grout are presented. Since grout can be considered as a fracture filling, although not naturally occurring, the same concept can be applied to study erosion of naturally occurring fracture filling. In Figure 4-8, the relationship between the hydraulic gradient and the shear stress is given for fracture apertures between 100 and 1,000 µm. This relationship is developed for plane-parallel and laminar flow. By analysing Figure 4-8, it can be concluded that the acting shear stress from flowing water generally is in the magnitude below 100 Pa but in large fractures and at high gradients it may become larger. However, it is unlikely to exceed 250 Pa (500 µm fracture). It should be noted that fractures above around 100 µm generally are easy to grout and hence will not be open during the construction phase.

The relationship in Figure 4-8 is derived for flow between smooth parallel plates. However, the flow in a rough rock fracture differs. The flow regime of a flowing fluid is determined by the Reynolds number, which describes the relationship between the inertia and the viscous forces. In a smooth pipe, the upper limit for a laminar flow is at a Reynolds number around 2,000. In a rock fracture, the rough surface leads to a lower critical boundary between laminar and turbulent flow. Experiments by /Cornwell and Murphy 1985/ examined the influence of fracture wall roughness on the flow regime. The result revealed that the Reynolds number for the flow regime transition was between 30 and 700. /Zimmermann 2005/ states that turbulent flow in a rock fracture can develop already at a Reynolds number of about 10. This means that, depending on the fracture roughness, the transition from laminar to turbulent flow occurs at a Reynolds number between 10 and 700, see Figure 4-9.

Laboratory experiments performed by /Axelsson 2006/ regarding the erosion of grouts show that the most important parameters are the groundwater flow regime and the relationship between the strength of the grout (considered as a fracture filling) and the erosive force from the groundwater. The study shows that the potential for erosion increases rapidly as the flow becomes turbulent and, hence, this is regarded as the most critical parameter.

Fracture filling

Regarding the minerals that are found in the fractures as fracture filling, it can be generally concluded that the weakest link is the bond between the fracture mineral and the surrounding rock. The strength of the fracture mineral in itself is higher than the bonding strength. Studies performed by /Khachadoorian 2003/ on the bond strength between mortar and different minerals showed bond strength values between 1.7 and 2.8 MPa when the mortar was cast on the mineral surface, see Figure 4-10.

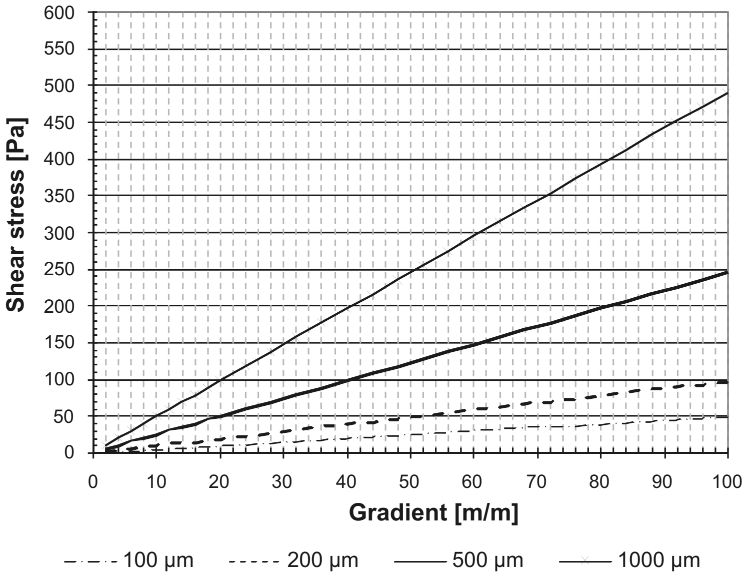

Figure 4-8. *The shear stress from water in different apertures and for different gradients. Modified from /Axelsson 2009/.*

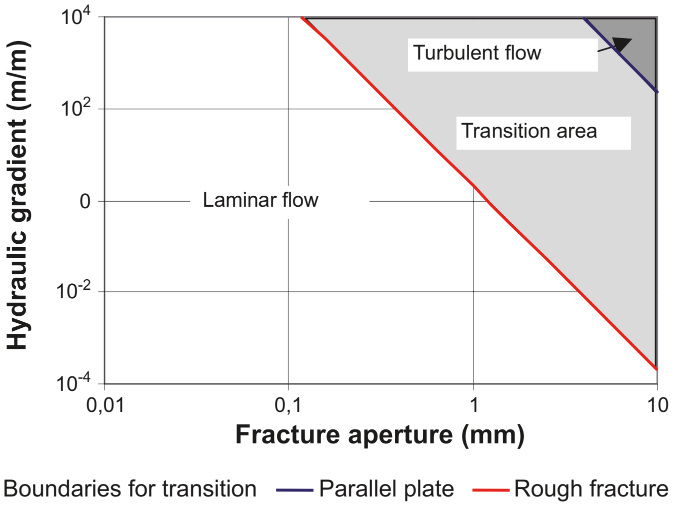

Figure 4-9. *Transition from laminar to turbulent flow in fractures of different apertures and hydraulic gradients. Modified from /Gustafson 2010/.*

Another common fracture filling material is clay, which is considered as a cohesive material. The strength of a cohesive material is dependent on the confining stress, a higher surrounding confining stress results in higher shear strength. This is, for instance, exemplified in general Quaternary clay where the strength increases with depth. Generally, the confining stress in a rock fracture at great depth can be assumed to be high, but as a worst case, the fracture can be in low stress and hence low confining stress which results in low shear strength. There are a number of studies reported regarding the shear strength of different clays, but not so many on the topic of the strength of clay as a fracture filling. However, by analysing results of measurements of the shear strength made on clay minerals, a magnitude of the strength of clay as a fracture-filling mineral can be estimated. /Olson 1974/ conducted consolidated undrained triaxial strength measurements on kaolinite, illite and montmorillonite. The conclusion from the test was that kaolinite generally has the highest strength followed by illite and the lowest strength was found in tests with montmorillonite. /Müller-Vonmoos and Løken 1989/ measured the strength of the same clay minerals with a ring shear apparatus. The samples were all consolidated to a normal stress of 100 kPa at a water content slightly over the liquid limit. These results also showed that the lowest shear strength was measured on the sodium montmorillonite. In the consolidated undrained triaxial tests on montmorillonite reported by /Mesri and Olson 1970/,

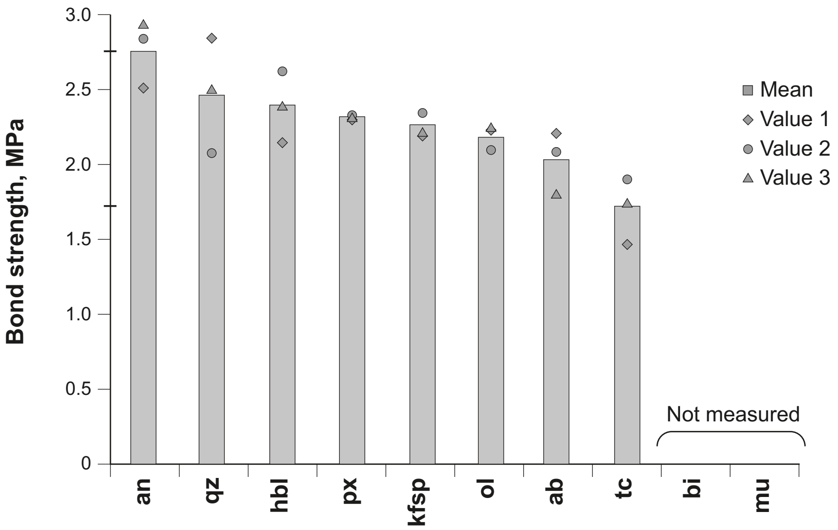

***Figure 4-10.** The bond strength between mortar and different minerals, from /Khachadoorian 2003/. The minerals are: an = anothite, qz = quartz, hbl = hornblende, px = pyroxene, kfsp = potassium feldspar, ol = olivine, ab = albite, tc = talc, bi = biotite and mu = muscovite.*

the lowest shear strength was measured for the sodium montmorillonite having a dry density of 2,650 kg/m^3, namely ≈10 kPa at an applied confining stress of 70 kPa. The shear strength did not increase greatly with increased confining stress for the sodium montmorillonite; at a confining stress of 450 kPa the shear strength was ≈ 40 kPa. Another series of studies have been reported by /Sridharan and Prakash 1999/, who conducted undrained shear vane tests on kaolin and bentonite with different water contents. The results show that the shear strength decreases with increasing water content. The shear strength for the bentonite was between 1.5 to 7 kPa (water content 150 to almost 475%) and for kaolin around 0.3–3 kPa (water content 45–80%).

As Figure 4-8 shows, the induced shear stresses caused by groundwater flow are orders of magnitude smaller than the shear strength of the clays after closure of the repository.

Fracture gouge

In order to examine the possibility of erosion of fracture gouge, the concept described by /Hjulström 1935/ can be applied, see Figure 4-11. The fracture gouge material can be considered to correspond to materials in non-cohesive beds and, according to Figure 4-11, this results in an erosive velocity of around 2 cm/s for grain sizes up to about 1 mm.

By assuming that the water flow in the fracture can be treated as the flow between parallel plates, the water velocity in the rock for different fracture apertures can be estimated according to Figure 4-12. The velocities are plotted for fracture apertures between 25 and 300 μm and hydraulic gradients between 0 and 10 m/m. The critical velocity for non-cohesive material, 0.02 m/s, according to Figure 4-11 is also marked in Figure 4-12. This means that at velocities faster than 2 cm/s, there is a large potential for erosion.

In natural conditions, the gradient is much smaller than ≈ 1, but around an excavated facility below the groundwater table the gradient increases and may become close to ≈ 1. However, the induced shear stresses caused by groundwater flow after the closure of the repository are orders of magnitude smaller than the shear strength of the clays.

Estimation of the erosion potential

The shear stress from laminar groundwater flow is generally low and generally does not exceed 0.1 kPa /Axelsson 2009/. However, as the roughness of the fracture increases, the potential for turbulent flow also increases and turbulent flow yields higher erosive forces.

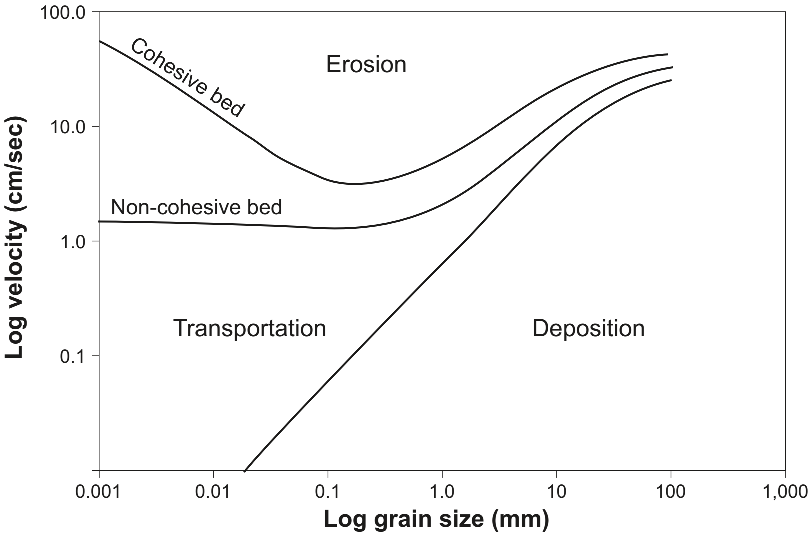

Figure 4-11. The Hjulströms diagram /Hjulström 1935/. For a non-cohesive bed, the erosive velocity is 2 cm/s up to a grain size of around 1 mm. The lower line in the diagram indicates the boundary between sedimentation and grains remaining in suspension.

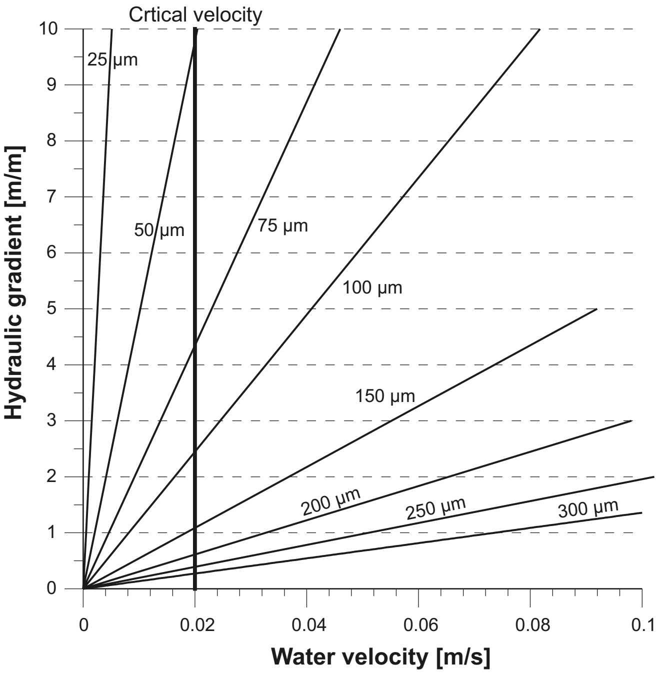

Figure 4-12. The water velocity as a function of hydraulic gradient and the fracture aperture.

The potential for erosion is low for most fracture fillings since the material strength is magnitudes larger than the forces exerted by the flowing groundwater. The same can be concluded regarding the bonding between the fracture filling and the surrounding rock. However, for clay minerals in the fracture there is a potential for erosion if the clay has high water content or if the confining pressure is low.

Regarding fracture gouge, there is a potential for erosion in fractures with an aperture of 150 µm at a gradient ≈ 1 and at lower gradients for fractures with larger aperture. Thus, during excavation, operation and initial saturation, there is a potential for erosion of fracture gouge due to the increased hydraulic gradient, see Figure 4-12.

4.6.5 Natural analogues/observations in nature

The process of erosion of sediments has been studied in sedimentology and dam hydraulics for a long time. Erosion has been investigated in sandstone fractures /Vilks et al. 1993/ and in a granite fracture /Vilks and Bachinski 1996/. The conclusion is that particles could be mobilised from the fracture surfaces by flushing. Because practically all water-conducting fractures have their walls covered by fracture-filling minerals, and clay is observed in many of these fractures, erosion may have had only minor effects. A similar problem, erosion of grout in fractures under high gradients, was studied by /Axelsson 2009/. The conclusion from that work is that it is only when tunnels are open that erosion may be a possibility.

4.6.6 Time perspective

The largest potential for erosion is during the initial stages of the repository life (excavation, operation and re-saturation periods). The fracture materials with largest erosion potential are clay minerals with high water content and fracture gouge. The potential increases with increased fracture aperture and increased hydraulic gradient. After saturation the potential for erosion is negligible.

4.6.7 Handling in the safety assessment SR-Site

Although during the excavation, operation and re-saturation periods there is always a potential for erosion in fractures, especially of fracture gouge and loose clay, grouting of the most transmissive flowing features will prevent this from happening. After closure of the repository, the hydraulic gradients during the temperate period will be so low that the potential for erosion is practically negligible. Although the gradients increase dramatically during glacial advance and retreat, the shear force is still very low.

Figure 4-13 shows the shear stress at the fracture/buffer interface as a function of the hydraulic gradient based on the output from hydrogeological modelling of the glacial case in SR-Site, see /Selroos and Follin 2010/. It is seen from the figure that even for a gradient as high as 10% and a fracture aperture as large as 1 mm, the shear stress is no more than 0.5 N/m^2. This could be compared to Figure 4-8 and Figure 4-12 that show that much higher gradients and, as a consequence of that, higher water velocities are required to cause erosion. The hydrogeological modelling of the "expanding ice front" case in SR-Site shows a similar picture.

Because of this, the erosion of materials in fractures is not evaluated in the SR-Site assessment.

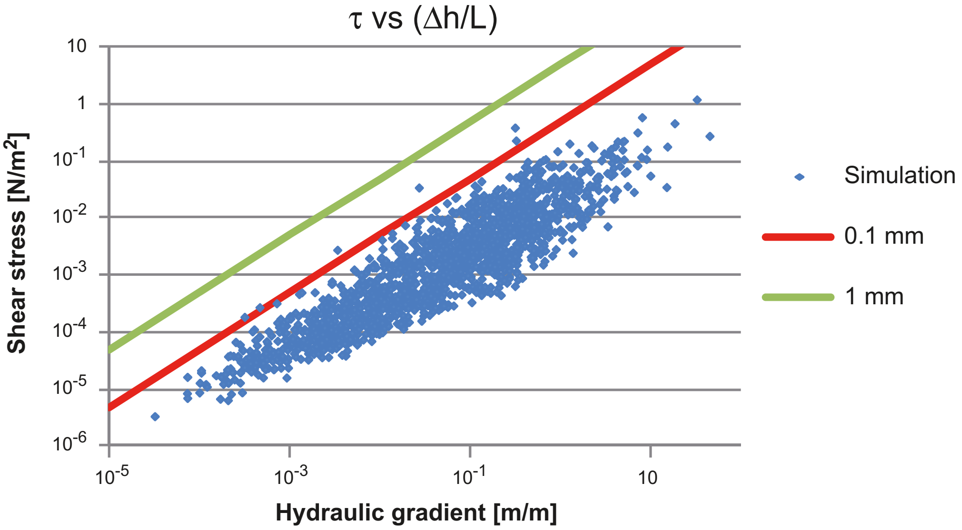

Figure 4-13. Shear stress at the interface between the bentonite gel that has intruded into a fracture and the water in the fracture as a function of hydraulic gradient and aperture /Selroos and Follin 2010/.

4.6.8 Uncertainties

Uncertainties in mechanistic understanding

The main processes are well understood and there are just minor questions to be answered, for instance how common is turbulent flow in the fractures around an excavated tunnel in Sweden?

Model simplification uncertainties in SR-Site

In the applied models described above there are some generalisations and simplifications regarding the water flow and the forces that can occur. However, the magnitudes are in the right order and the problems that can occur have been identified. Further modelling of this process is not judged necessary.

Input data and data uncertainties in SR-Site

Not relevant because the erosion of materials in fractures is not evaluated in the SR-Site assessment.

4.6.9 Adequacy of references supporting the handling in SR-Site

The references /Olson 1974, Müller-Vonmoos and Løken 1989, Mesri and Olson 1970, Sridharan and Prakash 1999, Vilks et al. 1993, Vilks and Bachinski 1996/ are peer-reviewed articles that have appeared in the open literature.

The reference /Selroos and Follin 2010/ is a SKB report for the SR-Site project that has undergone a documented factual- and quality review.

The references /Axelsson 2006, Axelsson 2009, Khachadoorian 2003/ are academic theses that have undergone peer review according to the Swedish academic system.

5 Chemical processes

5.1 Introduction

5.1.1 Overview

All processes that are not strictly thermal, hydraulic or mechanical are addressed in this chapter. In that sense the title “chemical” is somewhat misleading. Some processes, such as microbial activities, are clearly not only chemical, whereas other processes are at the borderline between physics and chemistry, such as radiation effects or earth currents. Specific aspects concerning radionuclide migration are discussed in Chapter 6.

Advection is the transport of solutes with groundwater flow. It is therefore intimately associated with hydraulics. The process of creating a mixture of two or more fluids is often denoted as “mixing”. Mixtures are mainly created by spatially variable advection and diffusion. Other processes that may be envisaged are matrix diffusion, tidal flows, etc. Often, it is the chemical aspects of groundwater mixtures that are of interest rather than the detailed “mixing” mechanism.

Classical chemical processes are: reactions in solution, surface complexation, ion-exchange, and dissolution/precipitation reactions, including solid solutions. These processes are discussed in Sections 5.4 (Speciation and sorption), 5.5 (Reactions groundwater/rock matrix) and 5.6 (Dissolution/precipitation of fracture-filling minerals).

The mathematical framework needed to model these processes is relatively simple, but quite extensive, and a detailed description is far from the scope of this report. Reactions in solution include the acid-base, metal-ligand and redox reactions that are described in chemistry textbooks at undergraduate level.

Most reactions in solution are in general fast (microseconds to minutes) and they are usually described by equilibrium expressions. On the other hand, many rock minerals are formed by cooling of molten rocks under high temperatures, and their precipitation from aqueous solutions at low “ambient” temperatures does not occur at all, because the solid phase is intrinsically unstable under such conditions. Often when such minerals react with water some of their constituents immediately precipitate in secondary insoluble solids, such as silicon, aluminium or Fe(III) oxides or hydroxides, and in some cases clays or zeolites are formed. This mineral transformation process is referred to as chemical “weathering” and in many cases it is quite slow, i.e. in the time frame of years to many thousands of years, depending on the composition of the water and on the flow regime.

Several redox transformations are also kinetically hindered at “ambient” temperatures and pressures. A typical example is the reduction of sulphate to sulphide. However, such a reaction may take place at elevated temperatures or pressures, e.g. in hydrothermal regimes, or it can be microbially mediated.

Redox processes are special in that they involve the transfer of electrons. Electron-rich species or systems are reduced or reducing, whereas electron-poor species or systems are oxidised or oxidising. For example, Fe^{2+} has one electron more than Fe^{3+} and, therefore, the former is reduced whereas the latter is oxidised. A more subtle example is CH_4 and CO_2, the former a reduced and the latter an oxidised form of carbon. Oxygen has a strong affinity for electrons, whereas hydrogen has a relatively low affinity for electrons. The consequence of this is that the distribution of electrons is in favour of carbon in the C-H bonds of CH_4, but concentrated towards oxygen in CO_2. Hence, carbon in CO_2 is electron-poor, that is, oxidised. Often reductants and oxidants, such as H_2 and O_2, are denoted electron-donors and electron acceptors, respectively.

Several redox processes are energetically favourable but kinetically hindered, as in the case of sulphate reduction. However, microbes are notorious in taking advantage of this fact. By using enzymes they can catalyse redox reactions while retaining some of the energy for themselves. However, this is only possible in systems that are in disequilibrium, that is, in systems where there is a simultaneous presence of an electron donor and an electron acceptor. Microbially mediated redox reactions are further discussed in Section 5.7.

The redox properties of a groundwater are important as they affect the redox state of metal ions. This is reflected in their electric charges, e.g. Fe^{2+}/Fe^{3+}, or U^{4+}/UO_2^{2+}. Large electric charges imply large electrostatic bonding with hydroxide ions, leading to hydroxide precipitation and low solubilities. A high electric charge also results in strong interactions with mineral surfaces (sorption) because these surfaces are normally electrically charged. In the examples mentioned above, Fe^{2+} and UO_2^{2+} are relatively more soluble and mobile in groundwater than their redox states Fe(III) and U(IV). Note, however, that reduced Fe(II) is more mobile than oxidised Fe(III), whereas the situation is reversed for uranium where oxidised U(VI) is more mobile than reduced U(IV). Speciation and sorption processes are further described in Section 5.4.

5.1.2 Geochemical conditions of the geosphere

The chemical situation in Swedish bedrock is generally very stable. Reaction and transport processes proceed continuously, but generally lead to changes only on a very long time perspective (thousands of years). Reactions occur between different components in the groundwater, between water and fracture minerals, and between water and the rock matrix. The groundwater flow results in transport of reactants and reaction products. The flow of groundwater also leads to mixing of different groundwater types from different regions of the geosphere.

The boundary conditions for the evolution of the chemical situation are given by inflow and outflow of water (with its dissolved components) from/to the biosphere, by exchange with very deep-lying groundwater and by the upward diffusion of geogases. In addition, the present-day geochemical situation, as well as transport and reaction processes in the geosphere, affect the geochemical evolution.

During the excavation and operation phases, the chemical situation close to the repository will undergo several changes. These are caused by increased infiltration of meteoric waters, upconing of deep saline waters, grout degradation, and possibly aeration of some parts of the rock.

In addition, large changes in the chemical composition of the groundwater are caused primarily by shoreline displacements and by long-term climate changes, which lead to altered infiltration of fresh waters and flow conditions, which in turn can lead to noticeable effects on the composition of the groundwater.

5.1.3 Temporal evolution

In order to be able to provide good estimates of future geochemical conditions, it is necessary to have an understanding of the past evolution, i.e. the conditions that have given rise to today's situation. The site descriptive models of the Forsmark area and the Laxemar subarea /Laaksoharju et al. 2008b, 2009a/ provide the current understanding of the historical evolution of geochemical conditions at these sites.

5.1.4 Importance for repository performance

In combination with the groundwater flow, the composition of the groundwater is of great importance for repository performance, both in the short and long term. The interaction between the engineered barriers and the groundwater determines how long the spent fuel will remain contained. Even in a situation where the containment has failed, the groundwater flow and composition are of importance as a determinant for the rates of dissolution and transport of radionuclides from the fuel.

The quantity of dissolved oxygen in the water and the quantity of sulphide that can come into direct contact with the copper canister are of importance for copper corrosion. These substances corrode the canister in different ways. Attack by oxygen may cause pitting, whereas sulphide corrosion is distributed evenly over the whole surface. Absence of oxygen at repository depth is, therefore, a requirement for the deep repository site. Other constituents in the groundwater do not affect the canister's integrity, except for a combination of extremely high salinity and low pH, which undermines the thermodynamic stability of copper metal.

For the buffer (bentonite), it is necessary that the groundwater contains a minimum of dissolved salts. The presence of divalent cations is essential for the bentonite not to form colloids (see Buffer, backfill and closure process report /SKB 2010e/). Very high salinities can significantly reduce the swelling capacity of the bentonite and thereby disable its function as a diffusion barrier between the canister and the rock. For the backfill, lower salinities are also of importance (see Buffer, backfill and closure process report /SKB 2010e/). Bentonite/aggregate proportions are, therefore, chosen with reference to prevailing salinities.

The pH and Eh of the groundwater are important for radionuclide transport. Under reducing conditions (no dissolved oxygen), many of the most radiotoxic nuclides occur in a reduced form with very low solubility. The solubility is lower at near-neutral pH than under acid or alkaline conditions. In groundwaters at planned repository depth in crystalline bedrock in Sweden, reducing conditions prevail and the pH is close to neutral. The total salinity of the water influences the retention of weakly sorbing radionuclides.

The water's content of colloids and microbes is also of great importance for radionuclide transport, since these particles can act as carriers for radionuclides. At high concentrations, strongly sorbing radionuclides will be able to adhere to colloids and microbes in competition with the retention on the fracture surfaces, and thereby they might be transported with the groundwater flow. In investigated groundwaters, the concentration of colloids has been so low that this transport mechanism is considered to be of no importance.

5.2 Advective transport/mixing of dissolved species

5.2.1 Overview/general description

Advection

Advection, i.e. transport with the flowing water, is the most important transport process for dissolved substances (solutes) in groundwater. Only a small portion of the volume of the rock is taken up by voids such as fractures and porous structures in the intact rock. The groundwater flows in these voids, but only through fractures and pores that are hydraulically connected and through that portion of the fracture and pore volume that is open to flow. The flow porosity, which is smaller than the total porosity of the rock, is the portion of the rock that is taken up by flowing groundwater. The total groundwater flow per unit area is called the Darcy flux. The mean transport velocity of the water particles, or any inert particle transported by the flowing water, is obtained as the Darcy flux divided by the flow porosity. This resultant transport process describes the bulk movement of the groundwater and is called advection.

Advection is of central importance for the chemical evolution of the repository. This is because it is responsible for transport to the repository of substances that influence the bentonite buffer and the canister, and because any releases of radionuclides from the repository can be transported to the biosphere by advection. Furthermore, advection is responsible for transport of reactants to and products from nearly all chemical and microbial reactions occurring in the geosphere. In this respect, advection is a driving force for dissolution of rock minerals, it affects the stability of fracture-filling minerals and grout, it drives microbial processes and methane hydrate formation, and it moderates the consequences of salt exclusion by freezing.

The Darcy flux is defined on a macroscopic scale. On smaller scales, velocity differences occur both within a fracture and between different fractures. These velocity variations lead to a mixing phenomenon called hydrodynamic dispersion. During transport in fractured rock, velocity variations between different flow paths are usually the main cause for dispersion. These flow paths are typically resolved by the groundwater flow models described in Section 3.1. The division of transport into an advective and a dispersive component is thus dependent on the scale studied and is relatively arbitrary. The advective component describes the mean transport, whereas the dispersive component takes into account velocity variations on scales smaller than that resolved by advection along different flow paths. Dispersion also contains a component that describes molecular diffusion in water. Dispersion is a model concept rather than an actual process.

As mentioned in Section 3.1, the groundwater fluctuates on short timescales as a result of, for example, tidal effects, rainfall events and seasonal variations (rainfall, storms at coastal locations, ground freezing and snowpack development). These short-term fluctuations are not relevant to the performance of a spent fuel repository in crystalline rock, which is only affected by the average flow system over periods of years.

It can be shown that a temperature gradient can cause solute migration (the Soret effect). However, in the context of the repository the magnitude of this process is normally much smaller than the transport of solutes due to advection, and it is, therefore, not considered further here.

Mixing

Mixing is a complex process involving both advection and diffusion which may vary both in space and time. Groundwater moves by advection in connected flow paths of the rock's fracture system. At flow path intersections, water from different conductive fractures is mixed. Advection thereby leads to a situation where different water types replace each other and/or are mixed. The mixing process may, in turn, be a driving force for other reactions such as dissolution or precipitation of fracture-filling minerals, colloid formation, etc. Mixing as a concept is frequently used in hydrogeochemical simulations of groundwater composition.

Evolution since the most recent ice age; After the most recent ice age, the different evolutionary stages of the Baltic Sea have influenced the mixing of groundwaters to a varying degree depending on the location in relation to the coastline. As the continental ice sheet advanced and retreated, glacial water penetrated down into the bedrock, displaced the previous water and mixed with it in the boundary layer, see Figure 5-1. It is not possible to set an exact limit today for how deep the glacial water reached, but significant proportions of water originating from colder climatic conditions have been found at 200 to 600 m depth at Forsmark and Laxemar /Laaksoharju et al. 2008b, 2009a/. Traces of such water are also found at greater depths. It is, however, unclear whether this water has the same origin, or whether it may derive from a previous deglaciation. This is especially the case in low conductive bedrock sections at Forsmark, i.e. in fracture domain FFM01 /Laaksoharju et al. 2008b/. However, it is assumed that the last glaciation had a significant impact on the present groundwater composition. Most of the groundwater from the previous deglaciations should have been flushed away if those earlier glaciations had similar evolutions to that of the last one.

At sites that at some time since the last glaciation have been covered by the sea, remnants of old sea water are generally observed /Laaksoharju et al. 2008b/. The driving force for the infiltration of sea water is its higher density, which has caused the water to penetrate down into the rock to a depth where the salinity was once equally high. The process of land uplift has since brought previously sea-covered sites above sea level, exposing them to inflow and outflow controlled by precipitation and topography.

Conditions at great depth; Highly saline water is usually encountered at great depth due to its higher density. However, the actual depth for these highly saline waters can vary from site to site. The salinity of the water exceeds that of the sea water, showing that its origin is either very saline water where the salt has been leached out of the rock over millions of years or saline water originating in seawater freezing, and there may even be an additional component of some ancient residual basinal brine.

Mixing is thus a process which is essentially controlled by external, climate- and land form-related conditions and which is of crucial importance for what changes can be expected to occur in the composition of the groundwater in the future. The obvious changes in composition are transitions between fresh water (meteoric water), saline water under permafrost, glacial meltwater and, in areas below the highest shorelevel, marine salt water, and brackish and fresh sea/lake water. Each type of water can displace the previous groundwater, alter equilibria and form or dissolve fracture-filling minerals.

There have been ten or so glaciations during the past million years, and, in consequence, probably some forty or so far-reaching changes of this kind. Each of these changes has left traces in the low-conductive parts of the rock where water exchange is slower than in the conductive zones, as discussed further under uncertainties.

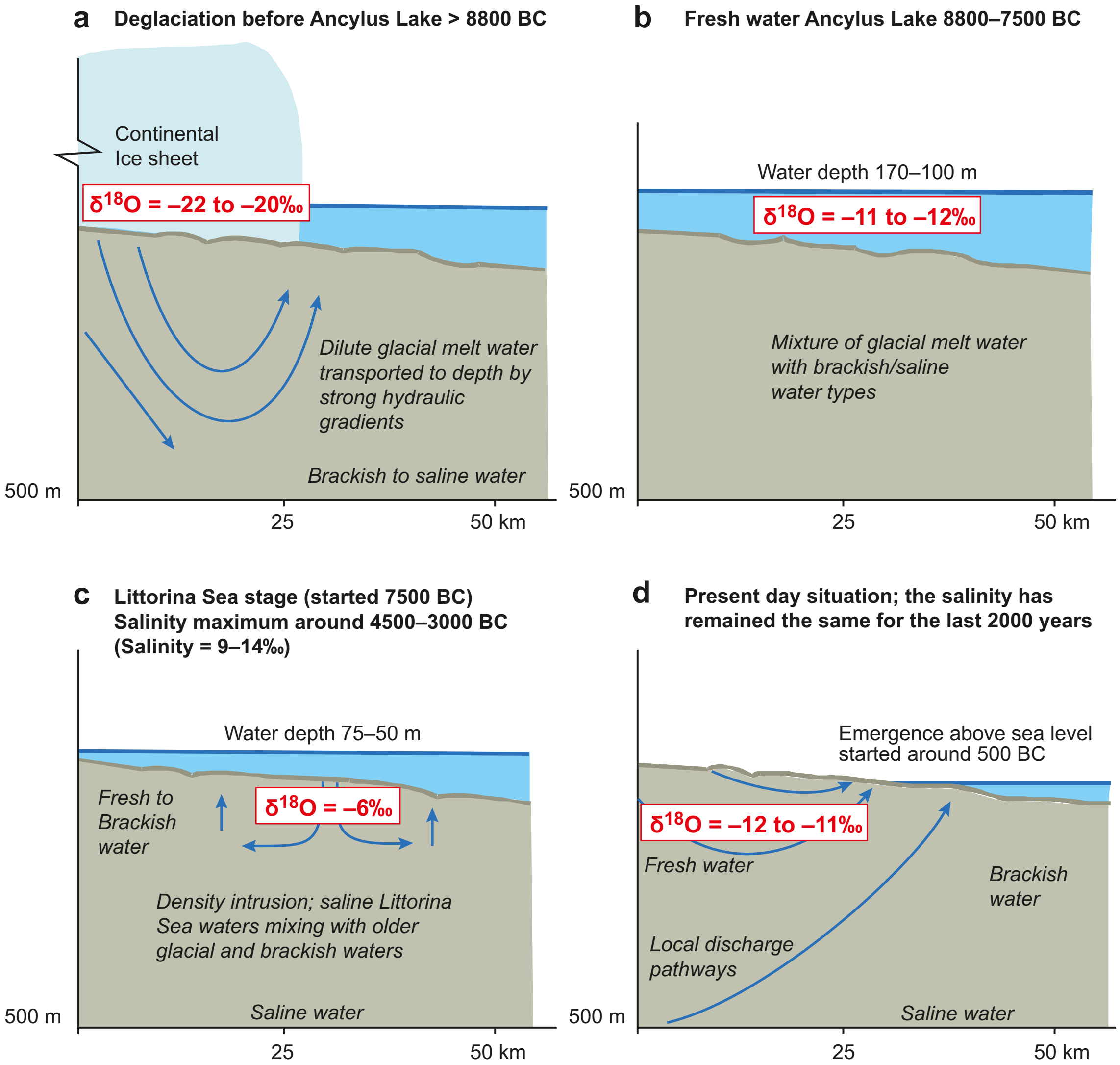

Figure 5-1. *Conceptual model for groundwater evolution in the Forsmark area from the retreat of the ice after the most recent ice age until today. The different stages of the Baltic Sea are of great importance for the large-scale groundwater flux at coastal sites. Blue arrows indicate possible groundwater flow pattern (Figure 2-17 in /Laaksoharju et al. 2008b/).*

5.2.2 Dependencies between process and geosphere variables

Table 5-1 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.2.7.

Table 5-1. Direct dependencies between the process "Advective transport/mixing of dissolved species" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Temperature in bedrock	No. But indirectly through groundwater flow.	–	–	No. But indirectly minor influence through flow of groundwaters with different temperatures.	–	–
Groundwater flow	Yes.	Excavation/ operation/ resaturation	Transport of salinity included in groundwater flow modelling (Section 3.1).	No. But indirectly by affecting groundwater composition (salinity).	–	–
		Temperate	Transport of salinity and reference waters included in groundwater flow modelling (Section 3.1). Flow field from hydrogeological modelling used in calculations of advective transport of radionuclides, see Section 6.1.			
		Periglacial Glacial	Transport of salinity from beneath a permafrost layer to repository depth included in groundwater flow modelling, see Section 3.1.			
Groundwater pressure	No. But indirectly through groundwater flow.	–	–	No.	–	–
Gas phase flow	No. But indirectly through groundwater flow.	–	–	No. But indirectly by changing groundwater composition (dissolved gas which may subsequently come out of solution).	–	See Sections 3.2 and 5.10.
Repository geometry	No. But indirectly through changes in groundwater flow induced by the repository geometry.	–		No.	–	–
Fracture geometry	No. But indirectly through groundwater flow.			No.	–	–
Rock stresses	No. But, indirectly if fracture apertures are affected.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Matrix minerals	No. Groundwater in the matrix is immobile.	–	–	No. Groundwater in the matrix is immobile.	–	–
Fracture minerals	No. But indirectly, precipitation of mineral phases (e.g. calcite) may cause clogging thus altering fracture aperture and groundwater flow.	–	–	No. But indirectly through reactions between constituents of flowing groundwater.	–	–
Groundwater composition	No. But indirectly through groundwater flow (density gradients).	–	–	Yes. Groundwater composition depends on advection and mixing of different constituents.	Excavation/ operation/ resaturation All other domains	Transport of salinity included in groundwater flow modelling, see Section 3.1. Distribution of salinity from hydrogeology modelling. Modelling of water composition based on output from hydrogeology modelling.
Gas composition	No.	–	–	No. But indirectly through groundwater composition by affecting concentration of dissolved gases.	–	See Sections 3.2 and 5.10.
Structural and stray materials	No. But indirectly as grouting alters groundwater flow and hence affects advection/mixing.	–	–	No. But indirectly through water composition since advection may transport constituents that will enhance corrosion of metals and degradation of cement.	–	See Section 5.8.
Saturation	No. But indirectly through groundwater flow.	–	–	No.	–	–

5.2.3 Boundary conditions

The exchange of solutes with the biosphere, with remote parts of the geosphere and with buffer/backfill in the repository comprises the boundary conditions for the advection and mixing processes. The waters from each of these sources will have a different composition.

Climate and shoreline changes will lead to changes in the composition of the water entering the geosphere, which in turn may lead to long-term changes in water composition at repository level.

5.2.4 Model studies/experimental studies

The advection-dispersion concept is often used in the modelling of solute transport, e.g. in simulating tracer tests. This concept expresses in its simplest one-dimensional formulation that the mass flux is given by the Darcy flux multiplied by the concentration in the aqueous phase plus the dispersion term given by the product of a dispersion coefficient and the concentration gradient. Often models applied to fractured rock also include matrix diffusion, which is discussed in Section 5.3. The advective and dispersive components, as well as matrix diffusion, are discussed in Section 3.1.

In modelling with the advection-dispersion concept, it has often turned out to be difficult to estimate parameters *a priori* for the advective and dispersive transport based solely on hydraulic data such as flow rates and pressures. Specifically, for estimating the timescale of the transport process, i.e. the travel time, also the flow porosity needs to be determined. Further, it has turned out that the dispersivity concept does not work generally at high spatial variability in fractured rock; among other things, scale dependence has been observed for the modelled dispersion. It is also noted that if other processes such as matrix diffusion are present, the effective porosity is greater than the flow porosity, and the effective transport velocity is slower than if the solute only accessed the flow porosity.

A number of combined studies have been done where experiments have been conducted in the field and modelled at the same time. In Sweden, experiments have, for example, been conducted in the Stripa Mine /Gnirk 1993, Olsson and Gale 1995/, in Finnsjön /Ahlbom et al. 1992/ and at the Äspö HRL /Gustafson and Ström 1995, Elert 1999, Winberg et al. 2000, Winberg et al. 2003, Poteri et al. 2002/.

The Forsmark and Laxemar/Simpevarp sites have been modelled within the site investigation programme of SKB, using models incorporating density driven flow, diffusive exchange of salt between flowing water and water in the rock matrix, and advection-dispersion, see e.g. /Hartley et al. 2005a, b, SKB 2005a, b, 2006a, Follin et al. 2008 and Rhén and Hartley 2009/. Groundwater chemical data have been analysed using, among others, mixing models /Laaksoharju et al. 2008a, b, c, 2009a/.

The importance of mixing in modelling the observed groundwater chemical compositions has long been a well established fact. However, quantitative results on the past evolution of an observed groundwater are more recent. Mixing is evaluated by means of inverse modelling, which involves starting from known results (measured data) and attempting to quantify the underlying processes, in this case mixing of groundwaters. A computer model for evaluation of hydrochemical data, called M3 /Laaksoharju et al. 1999b/, was developed with the aid of the data gathered in and around the Äspö HRL. Using this statistical multivariate analysis tool, it has been possible to conclude that a groundwater sample contains, for example, both a modern and a very old component simultaneously. Other codes have been developed that, in part, use mixing models to supplement geochemical reactions when accounting for observed groundwater compositions. For instance, the standard codes NETPATH /Plummer et al. 1994/ and PHREEQC /Parkhurst and Appelo 1999/ examine possible gas-water-rock reactions between components in the system and then, to satisfy mass balance requirements, they introduce elements or species that are not present in any of the selected phases, by mixing calculations.

The development of the M3 model during the evaluation of the hydrochemical conditions at Äspö, Forsmark and Laxemar has made it possible to calculate the proportions of different identified water types by reference to the components sodium, potassium, calcium, magnesium, chloride, sulphate, carbonate, deuterium, tritium and oxygen-18 /Laaksoharju et al. 1995b, Laaksoharju and Wallin 1997, Rhén et al. 1997, Laaksoharju et al. 2008a, 2009a/. The results indicate that mixing has occurred in several periods as a result of varying flow conditions. Mixing processes since the most recent ice age that have been identified and quantified are listed below (see also Figure 5-1).

1. Glacial meltwater penetrated to a depth of several hundred metres establishing an interface and partly mixing with saline groundwater, which was at least partly isolated from the atmosphere for millions of years.
2. Subsequently, Baltic Sea water from the Littorina stage (starting 9,500 years ago at Forsmark) sank down, due to its higher density as compared with glacial meltwater, until it reached saline water with the same or higher density. At this inversion, the glacial meltwater was pushed up into the conductive zones, but also remained in the low-conductive rock.
3. Meteoric water then gradually penetrated down to a depth of 100–200 m after rainwater started to infiltrate when Forsmark, Laxemar and Äspö rose above sea level. At Forsmark and Äspö this started about 2,500 and 8,000 years ago, respectively, whereas a large part of the Laxemar area was not at all submerged by the Littorina Sea transgression and, therefore, has been exposed to infiltration of meteoric water during the entire post-glacial period /Laaksoharju et al. 2008b, 2009a/.

This sequence of events probably occurred many times during past glaciation cycles. Most of the glacial meltwater in the rock was, most probably, washed out by lake, sea or meteoric waters during the temperate periods that followed. Therefore, any observed remnants of previous regimes in the fractures, e.g. glacial meltwaters, probably originate from the most recent event, i.e. the last ice age. However, some old dilute waters, previous to the last glaciation, have been found in the bedrock and their presence in the bedrock has been included in the hydrogeological simulations.

A hydrodynamic simulation of these conditions for the Äspö site has been carried out by /Svensson 1999/. Similar modelling has been performed for the Forsmark and Laxemar sites that have been investigated by SKB /Hartley et al. 2005a, b, Follin et al. 2005a, b, Follin et al. 2008, Rhén and Hartley 2009/. All the different water types that have occurred since the most recent deglaciation have been introduced under the pressures and other boundary conditions considered relevant. The transient simulation shows how different water types successively replace each other. For the Forsmark and Laxemar sites, the waters entering the system and eventually reaching depths of about 400 to 500 m in different proportions are: glacial meltwater (together with the remnant old dilute waters already present in the bedrock, at the start of the numerical simulation), Littorina Sea water (mainly in Forsmark) and, finally, in the case of Laxemar, today's meteoric water /Follin et al. 2008, Rhén and Hartley 2009/. Other analyses, which include dispersion, show that a remnant of previous water types should be traceable in the water chemistry, which agrees well with the hydrochemical data /Voss and Andersson 1993, Löfman and Taivassalo 1995/.

The comparison between simulation results and sampled groundwater compositions indicates that it is necessary to include all of the processes that influence water exchange in order to obtain a correct description. Interaction with low-conductive volumes and stagnant water reservoirs is of importance in determining exchange rates of the various waters.

5.2.5 Natural analogues/observations in nature

Several tools, such as the M3 computer model /Laaksoharju et al. 1999b, Gómez et al. 2006, Laaksoharju et al. 2008a, Gómez et al. 2009, Laaksoharju et al. 2009b/, as well as other statistical multivariate analysis tools and general geochemical reaction path codes, have been used to describe the hydrochemical mixing conditions in the analogue studies at Oklo and Palmottu /Laaksoharju et al. 1999a, Gurban et al. 1998, 2003/. In both of these cases, as at Äspö /Pitkänen et al. 1997, Laaksoharju et al. 1999c/ and many of the other Fennoscandian sites /Puigdomenech 2001, Pitkänen et al. 1998, 1999, 2004, Laaksoharju et al. 2008a, b, c, 2009a/, it has been possible to distinguish the major effects of mixing from the major effects of chemical reactions. The importance of mixing becomes apparent under the following circumstances.

1. The palaeo- and present climate has a huge impact on the hydrogeology and, hence, on hydrochemistry in Fennoscandia. This facilitates different water types (i.e. glacial, sea water and meteoric water) to enter or to be flushed out from the bedrock.
2. The temperature in the rock is relatively low and therefore most water-rock interaction processes are slow.
3. Where the groundwater flow is faster and more determining than reaction times (i.e. for highly transmissive conditions), the origin of the water may still be distinguished.

The significance of reactions becomes apparent, particularly with respect to: a) redox conditions where microbiologically mediated reactions are rapid, and b) pH and alkalinity values buffered by kinetically fast calcite precipitation/dissolution reactions /Gimeno et al. 2008/. In the model studies for Forsmark and Laxemar, the described flow conditions could subsequently be verified by hydrogeochemical models /Laaksoharju et al. 2008b, 2009a/.

As mentioned above, data from the site investigations at Simpevarp, Forsmark and Laxemar have been modelled for advection-dispersion, matrix diffusion and density driven flow, see e.g. /Hartley et al. 2005a, b, Follin et al. 2008, Rhén and Hartley 2009/, and groundwater chemical data have been analysed using, among others, mixing models /Laaksoharju et al. 2008a, b, c, 2009a/.

5.2.6 Time perspective

The timescale is determined by the timescale for shoreline displacement and other climate-related changes and by how long these changes continue to influence the hydrogeochemical situation.

The conditions within each domain of temperate, periglacial- and glacial conditions and their succession and duration control advection and mixing. For example, the ongoing glacial rebound, which is a result of the last glaciation, can lead to replacement of saline water with non-saline surface water. This can proceed for thousands of years at repository depth (500 m).

In a short time perspective, around 100 years, the groundwater disturbance caused by the repository will locally influence the groundwater chemistry to some extent.

5.2.7 Handling in the safety assessment SR-Site

The advection-mixing-dispersion process is included as an integral part of the evaluation of the hydrogeochemical evolution, see also Chapter 3 (Hydraulic processes).

The handling of radionuclide transport in groundwater by advection is described in Section 6.1.

The hydrogeochemical situation and the evolution of the groundwaters in the geosphere are modelled with respect to conceivable alterations of climate-related conditions. This is based largely on the knowledge that has been obtained by reconstruction of chemical and hydrological conditions in the past.

Excavation/operation/resaturation period

In Section 3.1, the groundwater flow modelling for the excavation/operation/resaturation period is described. Issues of specific relevance related to advection and mixing are upconing of saline water to repository depth and infiltration of fresh surface water to repository depth during the operation phase. The results, in the form of the spatial distribution of salinities, are used to estimate changes in the groundwater composition during the excavation/operation period.

Temperate climate domain

In Section 3.1, the groundwater flow modelling for the temperate climate domain is described. The results are of relevance to advection and mixing in the context of the hydrogeochemical evolution of groundwaters. The modelling not only produces the evolution of the salinity field, but gives also data on the transport and mixing of reference waters/water types.

Advection is a dominant process in the radionuclide transport calculations performed as part of the dose calculations. These simulations are described in Chapter 6.

Periglacial and glacial climate domains

During the remainder of the reference glacial cycle, i.e. during about 100,000 years, the assumed succession, duration and conditions within the periods of temperate, permafrost and glacial domains will control advection and mixing. As a consequence of wide variations in the hydraulic driving forces, groundwaters of various types will be mixed and thereby lead to dissolution and precipitation of e.g. calcite.

Qualitative and quantitative descriptions of extremes regarding hydrochemical conditions are made based on the climate domains (see SR-Site Climate report, Section 1.2 /SKB 2010c/).

In Section 3.1, the groundwater flow modelling for the periglacial and glacial periods is described. The main issues related to advection and mixing that are considered are the transport of highly saline water from beneath the permafrost layer to repository depth and the penetration of glacial meltwaters.

Of special importance during the glacial climate domain is the possible transport of oxygenated water down to repository level. The glacial conditions differ from today's situation in that there may be a lack of the soil cover that can contribute organic degradable material which bacteria can use to consume dissolved oxygen. The potential for oxygenated water to reach repository depth is assessed in SR-Site using transport resistances (F-factors) from the glacial hydrogeological modelling.

Earthquakes

No relation between earthquakes and advective transport/mixing of dissolved species in granitic bedrock have been identified. A build up of rock stress and its release will cause a change in hydraulic storativity and therefore induce a groundwater flow. This might be important in a system where solute transport is dominated by diffusion, but in the fractured rocks considered in SR-Site this effect may be neglected when compared with tidal and seasonal effects. It can also be assumed that local earthquakes can change the flow paths, for example due to gouge release in the fracture network. These changes are regarded to be minor since no large fracture faults that could induce larger changes in the mixing patterns of the groundwater are expected to be formed by earthquakes during the repository life time. Therefore, impacts of earthquakes on advective transport and mixing of dissolved species are not specifically handled in SR-Site.

5.2.8 Uncertainties

Uncertainties in mechanistic understanding

The conceptual uncertainties concerning advection/dispersion and mixing are small. Advection and dispersion are two well-defined model terms that are used, e.g. in calculating radionuclide transport in groundwater.

Model simplification uncertainties in SR-Site

Section 3.1 describes the model uncertainties concerning groundwater flow. The same uncertainties and simplifications apply to the transport of solutes by groundwater. Chapter 6 discusses model uncertainties and simplifications affecting the transport of radionuclides.

The uncertainties of the mixing modelling are evaluated in detail in /Gómez et al. 2006, 2009, Gimeno et al. 2008/. The exact quantification of the contribution from reactions versus mixing is complex, and at best semi-quantitative at the site scale. This requires different modelling approaches ranging through explorative analyses, mass-balance calculations, mixing calculations and coupled reactive transport modelling.

The results from mixing models that are used for hydrochemical modelling for a specific site are only valid for the site and conditions from which the data are derived. The predictive capability of the models used is thereby limited to the same geographic area or comparable areas where similar processes are active. The mixing models may also be used for predictions of future conditions assuming that chemical reactions (such as calcite dissolution/precipitation) do not significantly influence the overall composition of the groundwater mixture.

There are, however, such similarities in the data obtained from the Swedish sites that the reliability of the models can be considered good. In very generalised terms, the tritium and ^{14}C groundwater data indicate mean residence times of around hundreds to a few thousand years in the uppermost 100–150 m of the rock, whereas the residence time at 500 m depth lies in the range of thousands to tens of thousands of years, e.g. / Laaksoharju et al. 2008b, Laaksoharju et al. 2009a/. At greater depths, the residence times are generally much longer, see e.g. /Louvat et al. 1999/. At Forsmark and Laxemar, ^{36}Cl-data indicates residence times of at least several hundreds of thousands of years at depths larger than 600 m /Laaksoharju et al. 2008b, Laaksoharju et al. 2009a/.

The sequence in which different groundwater mixings have occurred represents a fundamental uncertainty in the interpretation of the mixing process. To this is added the degree of mixing (disturbance) caused by borehole drilling and sampling, which further complicates the situation (data uncertainty).

The mixing phenomena that have occurred recently can be quantified better and with greater certainty than those that occurred a long time ago. It is, for example, relatively simple to trace meteoric water that has infiltrated at Forsmark and Laxemar since the land rose above the surface of the sea, starting approximately 2,500 and 11,000 years ago, respectively /SKB 2008a, 2009a/. On the other hand, it is not possible from water sampling only to determine with certainty whether meltwater from the most recent ice age has reached down to a depth of only a few hundred metres, or much deeper, since water bodies may have been relocated due to the subsequent isostatic uplift.

Input data and data uncertainties in SR-Site

Section 3.1 describes the data uncertainties concerning groundwater flow. Chapter 6 discusses data uncertainties affecting the transport of radionuclides. The resulting uncertainties in the site descriptions that are used in SR-Site are discussed at length in the underlying site-descriptive modelling reports /SKB 2008a, 2009a/ and quantified in the SR-Site data report /SKB 2010b/ for use in SR-Site.

Waters from different parts of the fracture network are sometimes mixed during drilling and subsequent sampling. This mixing can incorrectly be interpreted as being representative of the point in the rock where the sample was taken. Under unfavourable conditions, the water may derive from a different location entirely or be mixed with different water types from many different fractures. By marking the drilling water, it is possible to make corrections for the quantity of water that has been injected during drilling. It is more difficult to correct for any disturbances caused by water from a fracture system flowing into the borehole and out into another fracture system. Careful evaluations have been carried out for the purpose of determining how representative the water samples are /Smellie et al. 1985, 1987, Smellie and Laaksoharju 1992, Laaksoharju et al. 1995b, Laaksoharju et al. 2004a, b, Smellie et al. 2008, Laaksoharju et al. 2008b/.

In addition to the uncertainty in representativeness, there are smaller uncertainties in measurements and analyses. These vary depending on analysis method, the constituents being analysed, interfering components, etc. The greatest uncertainties concern redox- and pH-sensitive solutes such as sulphide, iron, manganese and hydrogen carbonate, where the uncertainty in unfavourable cases may result in measured values being a factor 0.5–1.5 smaller/larger than the true value. The uncertainty for other analyses is less than a factor 0.9–1.1.

5.2.9 Adequacy of references supporting the handling in SR-Site

The references that support the process handling in SR-Site are /Laaksoharju et al. 2008a, b, 2009a/. /Laaksoharju et al. 2008a/ is a peer reviewed article that has been published in a scientific journal and the remaining two references are SKB reports that have undergone documented factual- and quality review.

5.3 Diffusive transport of dissolved species in fractures and rock matrix

5.3.1 Overview/general description

Liquid phase diffusion as a transport mechanism takes on importance where transport with the flowing water, advection, is small. Such conditions prevail in the pores of the rock matrix where there is no, or very little, water flow. Solutes transported with water flowing in fractures of the rock may enter these pores through diffusion, a phenomenon known as matrix diffusion /Neretnieks 1980/.

Matrix diffusion is one of the processes that has been addressed in the RETROCK project, aimed at examining how the retention and transport of radionuclides are, and should be, represented in the safety assessment models for deep geological repositories in fractured rock /RETROCK 2004, 2005/. The text of this section is an update of the corresponding text in the SR-Can geosphere process report /SKB 2006f/ which to a large extent is based on /RETROCK 2005/, and a report containing recommendations on matrix diffusivity and porosity data for SR-Can /Liu et al. 2006/. The integrated handling of matrix diffusion in radionuclide transport calculations is described in Section 6.1.

Matrix diffusion is a very important retention mechanism for solute transport in the geosphere, both for sorbing and non-sorbing radionuclides as well as for other dissolved species. For sorbing radionuclides, matrix diffusion gives access to the very large inner surfaces of the rock matrix where sorption can occur. These surfaces can typically be 3 to 6 orders of magnitude larger in area than the surfaces of the fractures where the water flows. For example, measurements of the surface area for major rock types of Forsmark by the BET (Brunauer Emmet Teller) technique /Byegård et al. 2008/ suggests internal surface areas on the order of 10^4–10^5 m^2/m^3, which should be compared to the flow-wetted surfaces mentioned in /SKB 2006d/ on the order of 10^{-1} m^2/m^3. For non-sorbing species, which may not be retarded by other processes than matrix diffusion, the access to stagnant porewater will to some extent retard the radionuclides. If a pulse release of non-sorbing radionuclide occurs from the engineered system, matrix diffusion may significantly lower the released peak activity to the biosphere. Such reduction may also occur in the case of radionuclides with sufficiently low half-lives that significant decay occurs during transport to the surface.

The key entities needed when assessing the diffusive properties of rock are the effective diffusivity D_e ($m^2\ s^{-1}$) and the storage capacity α (–) for the species in the rock matrix, and the connectivity of the porous system. For non-charged species that do not interact with the rock matrix, the effective diffusivity can be obtained from the product of the diffusivity of the species in free solution D_w ($m^2\ s^{-1}$) and the formation factor F_m (–) /Neretnieks 1980/. A prerequisite for this is that the characteristic length of the pores is much larger than the size of the species, otherwise size-exclusion effects may occur. For charged species, the diffusion may be decreased by ion exclusion or enhanced by surface diffusion /e.g. Olin et al. 1997, Axe et al. 2002/. The storage capacity of the rock matrix ($\alpha = \varepsilon + K_d\rho$) is the combined storage capacity available for dissolved species in the porewater and species sorbed on mineral surfaces. The key entity for storage of non-sorbing solutes in the porewater is the connected porosity ε (–). Matrix diffusion may occur in all types of connected porosity, including grain boundary pores, micro fractures, sheet silicate pores, and ruptured fluid inclusions /Möri et al. 2003a, Ota et al. 2003/.

Although there is a consensus among experts that matrix diffusion occurs in nature, there are still different opinions as to the depth to which diffusion can reliably be assumed to penetrate in the crystalline rock matrix. An entity crucial for the penetration depth is the pore connectivity. On one hand, there are arguments that support a large-scale pore connectivity on the metre scale or more /e.g. Bradbury and Green 1986, Möri et al. 2003a, Löfgren and Neretnieks 2006, Crawford 2008, Waber et al. 2009b /. On the other hand, *in situ* measurements have indicated small-scale pore connectivity of at least a few centimetres, showing that matrix diffusion under natural conditions occurs in rock directly in contact with water-conducting fractures /e.g. Smellie et al. 1986, Alexander et al. 1990, Heath et al. 1992, Miller et al. 1994, 2000/. A number of studies have been performed in the laboratory and in the field to increase the understanding of the extent of a connected pore space (see Section 5.3.4). Based on these studies, and the most recent research, the current position of SKB is that the microporous system can be connected on the decametre-scale. For example, the porewater studies carried out during the site investigations at Forsmark and Laxemar concluded that matrix diffusion occurred at least several decametres into the rock matrix /Waber et al. 2009a, b/.

Mineral surfaces of crystalline rock, such as granite, are most often negatively charged under natural groundwater conditions; thus there is a repulsion of negatively charged ions close to the surfaces /Stumm and Morgan 1996/. For very small pores, this means that anions are excluded from an important fraction of the pore space resulting in a smaller effective cross section area for diffusion and lower diffusion rates. Since matrix diffusion is the most important retention mechanism for anions, anion exclusion promotes transport of anions by advection in the water-conducting fractures through the geosphere. The importance of anion exclusion in crystalline rock is uncertain and the significance of this process has not been studied within the site investigations. However, in a SKB study performed subsequent to the site investigations on drill core samples from both sites, the effect of anion exclusion was found to be limited, at least at de-stressed conditions in the laboratory /Löfgren et al. 2009/. Furthermore, in a recent SKB investigation at the Äspö Hard Rock Laboratory, simultaneous matrix diffusion of anions, non-charged solutes, and cations has been studied in the undisturbed *in situ* rock matrix. The results from the LTDE-SD study suggest similar penetration depths of weakly sorbing cations and anions, indicating that the anion exclusion effect may exist, but is not overwhelming /Nilsson et al. 2010/. In the laboratory part of LTDE-SD, through diffusion tracer tests on 16 drill core samples were performed. In these tests, the non-charged tracer HTO and the anionic tracer iodide simultaneously diffused through the rock samples. The results indicate that the anionic tracer, on average, had a half an order of magnitude lower effective diffusivity than the non-charged tracer /Vilks et al. 2005/. In these measurements, the ionic strength of the background solution was set to fairly well match that of the *in situ* groundwater.

What can be suggested from measurements on Finnish granite is that the effect of anion exclusion is significant and reduces the effective diffusivity of anions by about one order of magnitude /Valkiainen et al. 1996, Olin et al. 1997/. According to electric double layer theory /e.g. Stumm and Morgan 1996/, the thickness of the electrical double layer is greater at porewaters of low ionic strength. Based on this, one can assume that the effect of anion diffusion increases with decreasing porewater salinity, if the pore throats are very narrow. In practice, however, it has been observed on Finnish granite that the dependence of anion exclusion on the porewater ionic strength is weak /Olin et al. 1997/.

Surface diffusion has been proposed as a process explaining observations of increased diffusion rates for some cations in crystalline rock /e.g. Ohlsson and Neretnieks 1998/. This means that sorbed radionuclides in the electrical double layer, both in the Stern layer and in the diffuse layer, may be affected by concentration gradients and thus be transported along the solid surfaces in a diffusion-like process. The phenomenon is well known in science and has been argued to be important for diffusion in bentonite buffers. However, its effectiveness in crystalline rock has not yet been commonly accepted. Thus, surface diffusion is usually neglected in safety assessments, which is regarded as a pessimistic approach, since an increased diffusivity in the rock matrix would increase the retention in the geosphere.

The stability of the matrix pore system over longer time periods is a crucial and difficult question. It has been shown that when applying pressure to a rock sample in the laboratory, the porosity decreases /e.g. Jacobsson 2007/ and so does the effective diffusivity /e.g. Skagius and Neretnieks 1986/. It is conceivable that the porosity will be slightly compressed *in situ* as a result of the ice load during glacial periods. The magnitude and importance of such potential compression remain to be investigated. Alterations in the flow field due to geological and climatic changes may affect the flow paths and thus also the contact area (flow-wetted surface) between flowing water and the rock matrix. This will in turn affect the retention capacity due to matrix diffusion. Precipitation and dissolution of mineral phases may, for example, be caused by changes in water composition from natural causes or by materials introduced in the repository. Changes in mineral phases, due to precipitation, dissolution, weathering, oxidation, and other alteration processes, may affect the available transport porosity both in the fractures and of the rock matrix.

Substantial areas within individual water-conducting fractures may contain effectively stagnant water. It has been suggested that if these zones are sufficiently large and accessible by diffusion from flow channels of limited width, the overall retardation effect may be some orders of magnitude greater than that predicted in their absence /Crawford and Sidborn 2009/. The retention capacity of the effectively stagnant fracture water is generally limited, although further diffusion from these regions into the rock matrix can provide much additional retention over longer timescales. Diffusion into effectively stagnant zones (which in a tracer test might be reasonably expected to include non-equilibrium diffusion between fast and slow moving flow streamlines) has been used to explain pronounced tailing in the breakthrough of short-term *in situ* tracer tests that could not be explained by diffusion into the rock matrix alone /e.g. RETROCK 2004, Neretnieks 2007/.

In addition to being of importance for radionuclide retention, matrix diffusion plays a role in the long-term evolution of hydrogeological and hydrogeochemical conditions at a potential repository site. A change in groundwater flow may occur through changes in water density, which in turn may occur as solutes diffuse between the flowing groundwater and the stagnant porewater (see Section 3.1). When estimating such changes in water density, by means of modelling salt diffusion in and out of the rock matrix, the D_e of the ion pair (e.g. Na^+Cl^-) should be used. Using the weighted harmonic mean of the D_w of the anion and cation when estimating the D_w of salt (see Equation 5-1) is generally accepted within the scientific community /CRC 2008/:

$$D_{w,salt} = \frac{\left(z_+ + |z_-|\right) D_{w,+} \cdot D_{w,-}}{z_+ D_{w,+} + |z_-| D_{w,-}} \qquad (5\text{-}1)$$

where z is the charge number of the ions. Here it is suggested that D_w can be replaced by D_e in Equation 5-1, although recognising that, to our knowledge, the grounds for doing this are not well described within the scientific community.

Exchange of solutes between the rock matrix and the flowing groundwater substantially affects the water composition. Concentration data for the major constituent chloride (and also considering $\delta^{18}O$), in porewater studies at Laxemar /Laaksoharju et al. 2009a, Waber et al. 2009a/ suggest that the freely flowing groundwater is fairly well equilibrated with the porewater in some locations at shallow levels to about 350 m. Inadequate data from Forsmark /Laaksoharju et al. 2008b, Waber et al. 2009b/ precludes a quantitative interpretation, but transient conditions are likely in the upper 150 m. At greater depths (about 500–600 m), transient conditions generally prevail at both sites. Transient conditions at these depths are not unexpected due to the complex historical evolution of the sites during past glacial cycles.

The discussion given in this section, as well as the modelling in SR-Site, is based on Fickian diffusion theory, even though it could be argued that the Maxwell-Stefan diffusion theory better handles multi-component mass transfer /Krishna and Wesselingh 1997/. However, as the concentrations of radionuclides are expected to be very low in the geosphere, it is judged that a multi-component mass transfer approach is generally not needed. Where there are sudden and major changes in the water composition, and thus extensive migration of groundwater species in the porewater, Fickian diffusion theory may be inadequate. However, even if it is conceivable that the groundwater composition may undergo major changes, also at repository depth, such changes will not be sudden, but take place over years to millennia. In short-term tracer tests, multi-component mass transfer effects cannot be ruled out, which should be kept in mind when evaluating the data.

5.3.2 Dependencies between process and geosphere variables

Table 5-2 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.3.7.

Table 5-2. Direct dependencies between the process "Diffusive transport of dissolved species in fractures and rock matrix" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Temperature in bedrock	Yes. But the variation is small in the expected temperature range.	All	Diffusion coefficients at constant temperature.	No.	–	–
Groundwater flow	No. But indirectly through groundwater composition (sustaining a concentration gradient between the water in the fracture and in the matrix porosity).	–	–	No. But indirectly through groundwater composition and density effects.	–	–
Groundwater pressure	Yes. But the effect is very small.	All	Diffusion coefficients at constant pressure.	No.		
Gas phase flow	No. But indirectly through water composition (dissolution of gas in water).	–	–	No. But indirectly through water composition (dis-solved gases which may subsequently come out of solution).	–	–
Repository geometry	No.			No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture geometry	Yes. Fracture/pore geometry influences the overall pathway for solutes – diffusing towards the fractures and also from the fractures into the rock matrix. An increase in fracture frequency enhances the area subject to diffusion.	Excavation/ operation	Site-specific descriptions of fracture and fracture zone geometry in groundwater flow modelling including diffusion of salt between mobile and immobile groundwater, see Section 3.1.	No.	–	–
		Temperate	As above for exchange of salt and reference waters in groundwater flow modelling. Geometry of flow paths and matrix porosity, see Section 6.1.			
		Periglacial Glacial	Site-specific descriptions of fracture and fracture zone geometry in groundwater flow modelling including diffusion of salt between mobile and immobile groundwater, see Section 3.1 Transport of radionuclides, discussed in Section 6.1.			
Rock stresses	No. But indirectly through changes in fracture/pore geometry.	–	–	No.		
Matrix minerals	No. But indirectly by acting as sorbing media and thereby affecting porewater concentrations or by changes in pore geometry.	–	–	No. But indirectly by affecting porewater concentrations and subsequent long term porewater – mineral interactions resulting in some alteration.	–	See Section 5.5.
Fracture minerals	No. But indirectly by acting as sorbing media and thereby affecting porewater concentrations or by changes in fracture/pore geometry.	–	–	No. But indirectly by changing groundwater composition that may induce precipitation-dissolution of minerals.	–	–

Variable	**Variable influence on process**			**Process influence on variable**		
	Influence present? **(Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence** **(How/If not – Why)**	**Influence present?** **(Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence** **(How/If not – Why)**
Groundwater composition	Yes. Concentration gradients are the driving force for diffusion.	Excavation/ operation	Exchange of salt between mobile and immobile water through diffusion included in groundwater flow modelling, see Section 3.1.	Yes. Diffusion affects the concentration of species in the groundwater.	Excavation/ operation/ resaturation	Effects on salinity of exchange of salt between mobile and immobile water included in the groundwater flow modelling, see Section 3.1.
		Temperate	Exchange of salt and reference waters between mobile and immobile water through diffusion included in groundwater flow modelling, see Section 3.1. Transport of radionuclides, see Section 6.1.		Temperate	Effects on salinity and reference waters of exchange of salt and reference waters between mobile and immobile water included in the groundwater flow modelling, see Section 3.1. Transport of radio-nuclides, see Section 6.1.
		Periglacial	Exchange of salt between mobile and immobile water through diffusion included in groundwater flow modelling see Section 3.1. Transport of radionuclides, see Section 6.1.		Periglacial	Effects on salinity of exchange of salt between mobile and immobile water included in the groundwater flow modelling, see Section 3.1. Transport of radionuclides, see Section 6.1.
		Glacial	See Periglacial above.		Glacial	Same as for periglacial above. Modelling of the effects of matrix diffusion on the consumption of oxygen present in infiltrating glacial melt waters.
Gas composition	No. But indirectly through dissolution of gas changing water composition.	–	–	No. But indirectly through water composition and degassing.	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	Yes. By affecting the pore space accessible to diffusing solutes.	All	Neglected; little significance compared with other influences.	No. Does not affect the water-saturation of the rock.	–	–

5.3.3 Boundary conditions

For the matrix diffusion process as such, there are no boundary conditions at the geosphere/biosphere interface or at the interface to the buffer and tunnel backfill to discuss. The relevant boundary conditions in this respect are those of the process that transport solutes over these boundaries, i.e. the boundary condition of the process advection. However, in order to treat the diffusion process quantitatively, the solute concentrations in the flowing groundwater in the fracture as well as the contact area between the flowing groundwater and the rock matrix, the flow-wetted surface, need to be expressed. The flow-wetted surface is strongly coupled to the flow conditions and, in integrated flow and transport modelling, the coupling between flow and retention by matrix diffusion and sorption is usually referred to as transport resistance (see further Section 6.1).

5.3.4 Model studies/experimental studies

The existence of an interconnected system of microfractures in granitic rock, where matrix diffusion may occur, has been verified by experiments both in the laboratory and in the field. A compilation of such studies is given in /Liu et al. 2006/. Furthermore, a compilation of the SKB field work on tracer tests from 1977–2007 is given in /Löfgren et al. 2007/. Recent evidence of large-scale pore connectivity comes from studies of the porewater salinity of the intact rock matrix, which suggests that the porous system is connected on at least the decametre scale /Waber et al. 2009a, b/.Some examples of studies of matrix diffusion are given below.

Laboratory experiments with the purpose of determining diffusion data in the matrix of crystalline rock have been reported by many researchers in countries like Sweden, Finland, the UK, Japan, Canada and Switzerland. Tracers penetrating through crystalline rock samples up to 12 cm in length have been observed /Löfgren and Neretnieks 2006/. Many of these experiments have been performed on undisturbed rock, but some have been performed on rock adjacent to fractures, fracture coatings and fracture filling material. These latter studies indicated that the porous media in or adjacent to fractures generally have higher porosities and diffusivities than the undisturbed rock /e.g. Byegård et al. 2002, Möri et al. 2003a, Byegård et al. 2008/. Results from re-stressed rock samples in the laboratory indicate that the effective diffusivity is lower in samples under stressed conditions /Bradbury and Green 1986, Skagius 1986/.

Field-scale tracer tests have been performed at a number of sites around the world. However, in most cases these have been carried out in the flowing water, focusing on obtaining a breakthrough curve and from inverse modelling extracting information on matrix diffusion. Only in a few cases, has overcoring been performed and direct evidence for matrix diffusion in the *in situ* rock matrix obtained. At 360 m depth in the Stripa mine in Sweden, such overcoring was performed and the tracer test resulted in diffusion profiles extending at least 40 cm into the undisturbed rock matrix /Birgersson and Neretnieks 1988, 1990/. The results also indicate large variability in the diffusivities evaluated from the experiments, despite a relatively homogeneous rock matrix. Tracers penetrating the *in situ* rock matrix beyond a few centimetres have also been observed in the Äspö Hard Rock Laboratory within the LTDE-SD programme /Nilsson et al. 2010/ and at the Canadian Underground Research Laboratory /Vilks et al. 2003/. These few *in situ* in-diffusion tracer tests show results that support the conceptual understanding of diffusion of solutes in the rock matrix.

Based on the analogy between diffusion and electromigration, as described by the Einstein relation, formation factors have been estimated from measurements of the rock resistivity and estimates of the porewater electrical conductivity /e.g. Skagius and Neretnieks 1986, Löfgren 2004, Crawford and Sidborn 2009/. Loggings of many boreholes have been conducted within the site investigation programme, both in the laboratory on drillcore samples /e.g. Thunehed 2007/ and *in situ* /e.g. Löfgren 2007/. The *in situ* results indicate that the unaltered rock has a micropore connectivity on at least the metre-scale. In addition, open fractures with stagnant water, and possibly also alteration zones around fractures, are found to increase the potential for migration. By comparing results from *in situ* and the laboratory, there are indications that the drillcore samples brought to the laboratory are stress-released and/or mechanically damaged, and might not be representative of *in situ* conditions /e.g. Crawford 2008/. See also /Waber et al. 2009b/ for an evaluation of perturbations on sample integrity by drilling and stress release.

5.3.5 Natural analogues/observations in nature

Natural analogues in the form of geological formations with elevated natural radioactivity (and even sites with normal background radioactivity) can be used to verify matrix diffusion as a process that took place over long time spans, compatible with the expected timescale of relevance for a repository. Analogues of this type, found for example at Kråkemåla in Sweden, Palmottu in Finland, Alligator Rivers in Australia and Cigar Lake in Canada, offer an opportunity to achieve better process understanding /Miller et al. 1994, 2000/. Measurements of concentration profiles in one fracture exposed in the Äspö tunnel and in a drillcore drilled from the surface have documented matrix diffusion of U and Cs on scales of some centimetres /Landström et al. 2001/. Concentration profiles from earlier uranium-series disequilibrium studies have been compared with model simulations /Rasilainen 1997/ showing that it is possible to get an idea of the effects of matrix diffusion. Agreement between measured and simulated profiles indicates that the matrix diffusion models used are realistic. Since the applied models include sorption processes, it can be claimed that the analogue studies also verify the fact that combined matrix diffusion and sorption are active processes *in situ*. The occurrence of an altered zone with higher porosity and larger volumes of secondary minerals may enhance matrix diffusion /Smellie et al. 1986, Landström et al. 2001, Andersson et al. 2002a/.

A common natural analogue is oxidation fronts in the crystalline rock matrix at hydraulically conducting fractures, where oxidising meteoric water from the surface infiltrates the reducing interior of the bedrock. Oxidising agents thereafter penetrate the rock matrix by molecular diffusion resulting in an oxidation front that may occur many decimetres from the fracture surface /RETROCK 2004/.

Within the site investigation programme, the concentration of solutes of the freely flowing groundwater, as well as of the porewater of the rock matrix, has been measured. Evaluations of the data /e.g. Laaksoharju et al. 2008b, 2009a, Waber et al. 2009a, b/ have provided concentration profiles of the major groundwater constituents that in general are predictable. Outliers that, without closer examination, may indicate rock volumes with a non-connected microporous system are rare, if at all existing. In /Laaksoharju et al. 2008b, Waber et al. 2009b/ it is proposed that the porewater of the target volume, i.e. the rock hosting the repository at depth at the Forsmark site is saturated with water infiltrating the rock before the latest glacial period. This proposal is substantiated with isotope considerations. However, considering the scarcity of hydraulically conductive fractures in the rock volume, this means that solutes observed in the porewater characterisations would have had to diffuse many metres, sometimes tens of metres, through the rock volume from the nearest flowing fracture. In /Waber et al. 2009a, b/ matrix diffusion was identified to occur over several decametres into the rock matrix, as shown by the quantitative description of Cl^-, $\delta^{18}O$ and δ^2H profiles in the porewater.

5.3.6 Time perspective

Matrix diffusion is a slow process. It is primarily the combination of matrix diffusion and sorption that gives the geosphere its retarding capacity. Even with advective travel times of a few tens or hundreds of years for transport from the repository to the biosphere, most radionuclides will be retarded by several orders of magnitude relative to the advective travel time. The exception is for non-sorbing or very weakly sorbing radionuclides, for which the effect of retardation is more pronounced on the peak release rates, in case of a pulse release, than on the radionuclide arrival times /SKB 2006b/.

5.3.7 Handling in the safety assessment SR-Site

Excavation/operation period

Diffusion of salt between mobile and immobile groundwater is included in the hydrogeological simulations carried out for conditions prevailing during operation of the repository, see further Section 3.1.7.

No radionuclide transport, and hence no matrix diffusion of radionuclides, is considered for the excavation/operation period, since the engineered barriers are assumed to be intact.

Temperate climate domain

The hydrogeological modelling undertaken for the temperate period represents variable-density flow due to variations in salinity. In this modelling, diffusion of several reference waters between mobile (flowing) and immobile groundwater is included, see Section 3.1. From the reference water mixture, the groundwater constituents, e.g. chloride, can be calculated. Thus, the groundwater flow modelling not only provides the groundwater flow conditions, but can also be used to explain e.g. slow changes in groundwater composition at great depth, e.g. from saline to non-saline (fresh).

Matrix diffusion is included in the modelling of radionuclide transport during the temperate period. It is of relevance during the whole period, and the influence of pore geometry and groundwater composition is implicitly considered in the selection of data, i.e. formation factor, porosity and diffusivities in unconfined water. The coupling to the advective transport of radionuclides in the fractures is handled via the flow-related transport resistance, see Section 6.1. Matrix diffusion is coupled to sorption via the concentration of the solute in the porewater which is handled by the K_d approach (see Section 5.4.7). The integrated modelling approach is further described in Section 6.1.7.

Periglacial climate domain

The exchange of salt between mobile and immobile groundwater is considered in the groundwater flow modelling carried out to study the groundwater flow patterns during permafrost conditions, see Section 3.1.7.

Matrix diffusion of radionuclides is considered in the simulations of radionuclide transport during permafrost conditions. The same approach as for the temperate period is used, but the different conditions are reflected in the selection of data, see also Section 6.1.7.

Glacial climate domain

The exchange of salt between mobile and immobile groundwater is considered in the groundwater flow modelling carried out to study the groundwater flow patterns during the advance and retreat of an ice sheet, see Section 3.1.7. In addition, penetration of oxygen (oxidised water) during a glaciation and reactions between oxygen and rock minerals are analysed, considering diffusion of oxygen into the rock matrix and subsequent reactions with rock minerals, see Section 5.5.7.

Matrix diffusion of radionuclides is considered in the simulations of radionuclide transport during glacial conditions. The same approach as for the temperate period is used, but the different conditions are reflected in the selection of data, see also Section 6.1.7.

Earthquakes

No relation between earthquakes and matrix diffusion has been identified.

5.3.8 Uncertainties

Uncertainties in mechanistic understanding

Diffusion/matrix diffusion is basically a simple process that can be well described and modelled and convincing evidence of its existence has been collected. According to /RETROCK 2005/, the main open questions concern the depth of connected porosity and whether the pore system is uniform and stable over long periods of time, so that constant diffusivities in the porewater can be assumed. Concerning the scale of the connected porosity, recent evidence /e.g. Löfgren and Neretnieks 2006, Crawford 2008, Waber et al. 2009a, b/ strongly suggest that the porous system of the repository host rock generally is connected on all scales relevant for a safety assessment.

Model simplification uncertainties in SR-Site

The main uncertainty related to matrix diffusion in the integrated modelling of radionuclide transport concerns the approach used to quantify the transport resistance. This is further discussed in Section 6.1.8.

In the modelling of radionuclide transport, matrix diffusion is considered for the host rock only, i.e. the presence of fracture-filling minerals and altered rock is neglected. Since experimental and *in situ* data indicate that matrix diffusion is higher in both altered rock and fracture fillings, this simplification, in principle, underestimates the retention capacity of the rock. In addition, surface diffusion effects are neglected.

High, but reversible sorption in altered rock and fracture fillings can possibly prevent radionuclides from getting access to the pores of the host rock. The implication of neglecting this potential effect in the modelling of radionuclide transport will be further evaluated, but the handling in SR-Site is as given above, i.e. to consider matrix diffusion for the host rock only.

A minor model simplification made in SR-Site radionuclide transport modelling is choosing a single constant value of D_w for all solutes. No correction is made for temperature, groundwater composition, or molecular diffusion coefficient of the individual solute. This is justified in the SR-Site data report /SKB 2010b/.

The main uncertainty related to matrix diffusion in the hydrogeological modelling is the same as in the radionuclide transport modelling, i.e. how to quantify the transport resistance, see Sections 3.1.7 and 6.1.8.

Input data and data uncertainties in SR-Site

Input data and associated uncertainties for quantifying matrix diffusion in the integrated radionuclide transport modelling are compiled in the SR-Site data report /SKB 2010b/. In addition to matrix diffusivity, the maximum penetration depths into the rock matrix and rock matrix porosity data are given and uncertainties in the data are assessed. The selection of data and the uncertainty assessment build on information from the site investigations, the site-descriptive models, recent SKB studies, and studies described in the open literature. Detailed references are provided in the SR-Site data report /SKB 2010b/.

5.3.9 Adequacy of references supporting the handling in SR-Site

In this section, references to a number of documents are made. These documents can be divided into three categories: peer-reviewed articles and textbooks; SKB reports; and reports from other organisations dealing with nuclear waste handling. The process of matrix diffusion is generally considered to be well described and uncontroversial within the scientific community.

For each process or entity discussed in this section, a main reference is listed and discussed in terms of qualification of references. Other documents referred to agree in terms of process understanding with this main reference. In cases where there are documents disagreeing with the main reference, this is highlighted when discussing the issue in other parts of this section.

Fickian diffusion is a very well known process that is described in numerous of text books /e.g. Stumm and Morgan 1996/.

Concerning the process of matrix diffusion the main reference chosen is /Neretnieks 1980/, which is a peer-reviewed article that is well known within the scientific community. This article agrees with numerous of other peer-reviewed articles and textbooks.

Concerning the issue of accessibility of dissolved species to the different types of pores within the *in situ* rock matrix, /Möri et al. 2003a/ is chosen as the main reference. This is a well written report from Nagra, where experimental methods and conclusions are transparently described. Furthermore the experiment is performed on relevant rock types. The report is also summarised in the peer-reviewed article /Ota et al. 2003/.

Concerning the issue of long-range pore connectivity, /Löfgren and Neretnieks 2006/ is chosen as the main reference. This is a peer-reviewed article presenting results from experiments performed on rock samples from the Laxemar site. The article also discusses the debate within the scientific community, concerning whether the porous system is connected on a limited scale or on a large scale *in situ*. The suggestion of long-range pore connectivity is supported by evaluations of porewater compositions /Waber et al. 2009a, b/, which are SKB reports that have undergone documented factual review.

Concerning the issue of anion exclusion, /Olin et al. 1997/ and /Vilks et al. 2005/ are used as the main references. /Olin et al. 1997/ is a well written report from Posiva, which presents both theory and experimental research results. Both methods and conclusions are transparently described. Furthermore, the experiments are performed on relevant rock types. /Vilks et al. 2005/ presents experimental results from the laboratory part of LTDE-SD, including results from studies of simultaneous diffusion of non-charged and anionic tracers in rock samples from the Äspö Hard Rock Laboratory. This rock has, in the site investigations and other studies, been shown to have similar matrix diffusion properties as rock from the Forsmark site. Interaction between charged species and the mineral surface is frequently discussed within peer reviewed articles /e.g. Axe et al. 2002/ and textbooks /e.g. Stumm and Morgan 1996/.

Concerning the dependence of *in situ* stress on the matrix diffusivity, /Skagius and Neretnieks 1986/ is used as the main reference. This is a peer-reviewed article that is well known within the scientific community. The experiments presented are performed on relevant rock types.

The analogy between diffusion and electromigration is described by the Einstein relation, which is discussed in numerous textbooks and peer-reviewed articles. In the peer-reviewed article /Löfgren and Neretnieks 2006/ the analogy is discussed in the context of crystalline rock.

5.4 Speciation and sorption

5.4.1 Overview/general description

The term "sorption" is a broad concept that describes the processes by which dissolved solutes are sorbed (adsorbed or absorbed) on or in another substance /IUPAC 1997/. In the context of radionuclide transport processes relevant for safety assessment, however, adsorption of dissolved species to mineral surfaces by way of electrostatic and covalent chemical bonding (surface complexation) are mainly considered. Transported radionuclides are frequently in the form of ionic, charged species and will tend to sorb on mineral surfaces that possess a net charge of opposite sign. Such interactions are well described in the scientific literature /e.g. Stumm and Morgan 1996/ and the most important mechanisms for this interaction are considered to be ion-exchange (a purely electrostatic adsorption process) and surface complexation (involving covalent bonding to chemically reactive surface groups).

Sorption can take place directly on the outer surfaces of flow-bearing fractures or on grain-boundary surfaces and microfractures within the rock matrix, where the porewater is effectively stagnant. Sorption can also take place on other materials, such as secondary clay minerals in fracture-surface coatings. Generally, sorption processes result in the retardation of radionuclide transport along a flowpath, although when radionuclides sorb on mobile solid materials such as colloids, the effectiveness of the retardation may decrease. There are other processes apart from sorption, such as precipitation and co-precipitation, which can give rise to additional retardation effects for transported radionuclides. However, owing to the difficulties in adequately quantifying and modelling these processes, they are not usually considered to contribute significantly to retardation in safety assessments.

The consideration of mineral precipitation/dissolution and the formation of solid solutions (i.e. co-precipitates) is, however, crucial for establishing relevant background concentration ranges for stable and naturally occurring radioactive isotopes which can influence the sorption of their radioactive, repository derived counterparts. This is particularly important for solutes such as cesium, strontium, and uranium. Consideration of the background concentrations of stable and naturally occurring radioactive isotopes is important for assessment of sorption properties owing to the frequently non-linear nature of radionuclide sorption isotherms. In the case of radium, natural background levels of the radionuclide are sufficiently high that this largely determines the concentration range in which sorptivity of the nuclide is to be assessed. Co-precipitation of radium and barium as a solid solution in barite is well known and, under most environmental conditions, is expected to exert an important control on the concentration range of radium present in groundwater owing to the low solubility of barite and its ubiquitous nature /Bruno et al. 2007/. Although such processes are carefully considered during the selection of K_d data, no attempt is made to attribute additional retention in the geosphere transport modelling arising from these processes on account of the difficulty of demonstrating that they provide a reliably quantifiable retardation effect.

Depending on the process in question, the strength of the sorption is highly dependent on the chemical properties of the individual ions and the presence of complexing agents and other dissolved solutes in the groundwater that may compete for sorption sites. It is, therefore, essential to know the redox conditions, groundwater pH, and concentration of complexing agents, such as carbonate, in order to predict sorptivity. Certain radionuclides (e.g. radioisotopes of uranium, neptunium and plutonium) are sensitive to redox conditions, whereas others (e.g. cesium, strontium, and thorium) are generally insensitive to the redox conditions in the groundwater. For the radionuclides that exhibit such sensitivity, the chemical valency of the dissolved radionuclide is controlled by the redox state of the groundwater, which has a direct impact on its propensity to form chemical bonds with mineral surface groups and undergo surface complexation.

Complexation in the aqueous phase can reduce the sorptivity of some radionuclides, although in other instances the sorptivity can actually be increased (e.g. bidentate sorption of uranyl carbonato complexes /Bargar et al. 1999/). The magnitude of the effect depends upon the chemical properties of the radionuclide concerned and the types of complexing agents present and their properties. The solution chemistry of simple complexing agents, such as dissolved carbonate, is well described theoretically and can be accounted for with relative ease in the aqueous phase. However, the impact on sorptivity when participating in sorption reactions is often less well characterised. The presence of dissolved carbonate, for example, can have complex direct and indirect effects that are difficult to predict *a priori* (included here are direct effects such as the formation of ternary surface complexes with radionuclides as well as indirect effects such as possible shifting of the mineral surface point of zero charge related to carbonate sorption /e.g. Stumm 1992/).

More complex ligands such as humic and fulvic substances can also be accounted for, although they are generally associated with decay of cellulosic organic materials and are thus of more concern in a near-surface environment. Bacterial siderophores, which can bind metals strongly, are typically only produced by bacteria under aerobic conditions where the availability of Fe(III) is low. At repository depth, these substances are considered to be of only limited importance. In connection with ion exchange, the salinity of the water is of great importance. High salinity reduces the sorption of, for example, cesium and strontium by way of competitive effects, involving ion-exchange sorption of other cations in the groundwater.

The different minerals participating in sorption reactions have different capacities for the adsorption of radionuclides. Clay minerals and iron oxyhydroxides, for example, have a large capacity to bind radionuclides, whereas quartz and feldspar tend to sorb very weakly. In granitic rocks, it is typically dark minerals such as biotite, its alteration product chlorite, as well as hornblende which are thought to have the strongest affinity for sorption of radionuclides. The sorption of cesium and strontium, for example, is known to be strongly concentrated to biotite and chlorite (micas) which, being phyllosilicate minerals, have a large interlayer capacity for ion-exchange sorption /e.g. Torstenfelt et al. 1982, Huitti et al. 1998/. Uranium and neptunium also have an affinity for the iron-rich dark minerals /Kienzler et al. 2009/, possibly due to surface complexation sorption on frayed edge sites of micas combined with reduction to the more strongly sorbing tetravalent state in the presence of ferric oxide alteration products. The surface complexation sorption of nickel, plutonium and americium, on the other hand, appears to be less specific, although autoradiographic studies do suggest heterogeneous distribution of sorption /Pinnioja et al. 1984/ with sorption concentrated on minerals possessing high surface areas, such as biotite/chlorite and hornblende.

Although sorption of radionuclides is generally reversible in a thermodynamic sense, the incorporation of radionuclides into mineral lattices can result in an effectively irreversible immobilisation of the radionuclide. However, owing to the dynamic equilibrium of most common mineral phases likely to incorporate radionuclides, irreversible immobilisation is not always verifiable, and such retardation processes are usually neglected in safety assessment.

Although the master variables pH, redox, and concentration of complexing ligands in the groundwater largely determine the speciation (distribution of an element amongst different chemical species) of radionuclides, temperature and pressure also play a minor role by way of the effect that these variables can have upon the thermodynamics of chemical reactions. The importance of chemical speciation lies in its impact on the geochemical immobilisation reactions likely to occur and their consequences for radionuclide mobility.

5.4.2 Dependencies between process and geosphere variables

Table 5-3 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.4.7.

Table 5-3. Direct dependencies between the process "Speciation and sorption" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. A temperature dependence exists (2nd and 3rd laws of thermodynamics).	Excavation/ operation	Process neglected for radionuclides since engineered barriers are intact.	No.	–	–
		Temperate Periglacial Glacial	Use of K_d approach. Temperature effects are neglected owing to lack of internally consistent data sets for chemical reactions of sorbing radionuclide species.			
Groundwater flow	No. But indirectly by affecting water composition.	–	–	No.	–	–
Groundwater pressure	Yes. Affects chemical speciation, solubilities of gases and minerals.	All	Influence neglected; little significance compared with other influences.	No.	–	–
Gas phase flow	No. But coupled through groundwater flow.	–	–	No.	–	–
Repository geometry	No.	–	–	No.	–	–
Fracture geometry	Yes. Fracture aperture determines surface retardation coefficient (and access to matrix for subsequent sorption).	Excavation/ operation	Process neglected for radionuclides since engineered barriers are intact.	No. Only if precipitation is considered, aperture could be changed.	–	–
		Temperate Periglacial Glacial	Geometry of flow paths, see Process 6.1. Site-specific porosities, BET surfaces and stress effects considered in the selection of K_d. Surface retardation neglected.			
Rock stresses	No. But indirectly through changes in fracture/ pore geometry.	–	–	No.		
Matrix minerals	Yes. Mineralogy important for sorption mechanisms.	Excavation/ operation	Process neglected for radionuclides since engineered barriers are intact.	Yes. Precipitation/co-precipitation may change matrix properties when trace elements are incorporated into matrix mineral structure (lattice).	All	Effect neglected (precipitation effects not accounted for), see Section 5.4.7.
		Temperate Periglacial Glacial	Site-specific minerals and BET surfaces considered in the selection of Kd values.			

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture minerals	Yes. Mineralogy important for sorption mechanisms.	Excavation/ operation Temperate Periglacial Glacial	Process neglected for radionuclides, since engineered barriers are intact. Site-specific minerals and BET surfaces considered in the selection of K_d values. However, surface retardation neglected.	Yes. Precipitation/co-precipitation may change fracture surface properties when trace elements are incorporated into mineral structure. Also influences groundwater composition affecting sorption.	All	Direct effects neglected (precipitation effects not accounted for). Also, sorption on fracture surfaces not accounted for, see Section 5.4.7. Mineral equilibrium is considered for establishing background concentration ranges of competing solutes.
Groundwater composition	Yes. Speciation, pH effects, salinity effects etc.	Excavation/ operation Temperate Periglacial Glacial	Process neglected for radionuclides since engineered barriers are intact. pH, redox, complexing ligands, salinity (ionic strength), organic acids, microbes considered in the selection of K_d values.	Yes. Uptake of trace elements controls concentration in water phase.	Excavation/ operation Temperate Periglacial Glacial	Process neglected for radionuclides. Sorption of radionuclides and trace elements not accounted for when main elements determined. For radionuclides, see Section 6.1.
Gas composition	No. But indirectly through dissolution of gas changing water composition.	–	–	No. But indirectly since water phase and gas phase concentrations are related by thermodynamic relations.		
Structural and stray materials	Yes. Sorption may take place on cement materials. Also indirectly since their degradation can influence groundwater pH and create secondary minerals in fractures, organic ligands etc.	All	Effect not considered.	No.	–	–
Saturation	Yes. By affecting the surfaces accessible to sorption.	Excavation/ operation Temperate Periglacial Glacial	Process neglected for radionuclides since engineered barriers are intact. Sorption of radionuclides considered for saturated conditions only.	No.	–	–

5.4.3 Boundary conditions

Boundary conditions are not relevant for the process in question, given how it is treated in the safety assessment, see below.

5.4.4 Model studies/experimental studies

Sorption of aqueous species on solids can be quantified empirically using a K_d approximation or described using mechanistic modelling approaches. The K_d concept simply describes the partitioning ratio of sorbed to dissolved solute without any specific consideration of reaction mechanisms or speciation. More elaborate, isotherm-based approaches attempt to capture non-linearities of sorptivity with changes in solute surface loading and competitive effects, although are still based upon largely empiric reasoning without reference to specific sorption mechanisms. Mechanistic modelling approaches are based upon a thermochemical formulation (thermodynamic sorption models, or TSM's). Surface-complexation and ion-exchange models fall into this latter category.

Sorption of a number of radionuclides (isotopes of Cs, Sr, Am, Ra, Ni, U, Np) has been studied as part of the transport properties site investigations at Forsmark and Laxemar /SKB 2008a, 2009a/. Other experimental, radionuclide-specific studies of sorption are reported in the literature and have been used for previous compilations of sorption properties /e.g. Crawford et al. 2006, Carbol and Engkvist 1995, Stenhouse 1995, Hakanen and Hölttä 1992/. These are usually conducted as batch tests, where a radionuclide spiked groundwater sample or simulated groundwater specimen is contacted with a geological sample (usually crushed) for a period of time ranging from days to months until an approximately equilibrium state is reached. Rock samples and water compositional ranges are chosen to represent the typical spatial variability for the repository site (usually this reflects a range of pH levels, redox states, ionic strengths and radionuclide concentrations). The change in the aqueous concentration of the radionuclide relative to its initial concentration provides an indication as to the extent of sorption. Column tests with flowing water can also be used to estimate the sorption, although interpretation is additionally complicated by the need to simultaneously account for more complex transport processes. In the field, attempts have been made to estimate sorption directly by determining the distribution of a tracer between fracture surfaces and equivalent groundwater in boreholes /e.g. Landström and Tullborg 1990/ although interpretation is difficult. Transport experiments with sorbing tracers in the field can also be used to estimate the strength of the sorption process /e.g. Löfgren et al. 2007/. In addition, sorption properties can be evaluated from in-diffusion and through-diffusion experiments in intact rock pieces, e.g. /Byegård et al. 1998, Widestrand et al. 2010/.

Provided the sorption is an approximately linear, reversible process, a distribution coefficient, K_d, for the particular water chemistry in question can be estimated. The assumption of linearity is usually satisfied at the low radionuclide concentrations that are of interest, or otherwise incorporated in the overall range of uncertainty estimated for the K_d value, and the assumption of equilibrium is met if the sorption process has a characteristic timescale that is much shorter than the timescale for advective transport. The use of K_d entails a simplification of what is, in reality, a very complex set of processes. Models that take into account non-linear sorption or non-equilibrium conditions exist, although they are seldom used in safety assessments owing to difficulty of implementation in an adequate fashion.

5.4.5 Natural analogues/observations in nature

Sorption as a reversible equilibrium process is difficult to observe directly in nature in an unambiguous fashion owing to the very low immobilised concentrations characterising the process. However, other immobilisation processes, such as precipitation, are easier to observe macroscopically and can be readily studied in geological samples. Examples include the natural analogues (specifically uranium oxide precipitation at redox fronts) at Poços de Caldas, El Berrocal, Cigar Lake, Grimsel and the "fossilised" ancient nuclear reactor at Oklo /Miller et al. 2000/. Coprecipitation of radionuclides with calcite, barite, and cement-derived phases is well known and has been studied extensively. The state of the art concerning solid solutions of interest in nuclear waste management can be found summarised in /Bruno et al. 2007/. A compilation of studies on natural analogues regarding the mechanisms controlling the aqueous concentrations and speciation of several elements is given in /Bruno et al. 2002/.

Sorption can, in principle, be studied by examining the immobilisation of tracer solutes within rock samples retrieved in post-mortem evaluations of tracer experiments. The excavation of the rock volume involved in tracer tests can also be performed in conjunction with resin injection which allows the flowspace structure to remain intact thereby giving additional information concerning fracture aperture and porosity distributions (see e.g. /Möri et al. 2003a/ and the review of SKB related tracer studies in /Löfgren et al. 2007/).

5.4.6 Time perspective

For most radionuclides, sorption processes are considered to be very fast compared with the timescale for advective transport in fractured rock. This means that dynamic sorptive equilibrium between the rock and aqueous phase can be assumed to prevail under natural conditions. Processes that lead to incorporation of radionuclides in mineral lattices are much slower than ion exchange and surface complexation and cannot always be considered to be in an equilibrium state. However, these processes are not relied upon directly in the safety assessment and may be considered to be processes that give rise to additional, although unquantified, retardation (see below).

5.4.7 Handling in the safety assessment SR-Site

Excavation/operation period

During the excavation and operation period of the repository, the system is characterised by the tunnels being at atmospheric pressure. Also, the re-saturation phase of the repository is included in this period, when the backfilled tunnels go from zero to full saturation.

No radionuclide transport is expected to occur during this phase.

Temperate climate domain

For sorption, it is assumed that a simplified linear equilibrium model (constant K_d) is applicable for safety assessment. This approach implies that geochemical conditions are sufficiently time invariant that the simplified modelling approach is valid and that retention processes such as surface precipitation and co-precipitation are not considered to contribute towards retardation in the safety assessment.

In order not to overestimate sorption in connection with possible changes in water chemistry, cautiously pessimistic distribution coefficients are assigned /Crawford 2010/. In SR-Site, K_d values for ion-exchanging solutes are derived for site-specific conditions (i.e. different major ion compositions) as defined by hydrogeological/hydrogeochemical modelling. For radionuclides that sorb principally by way of a surface complexation mechanism, best estimate K_d values are provided for the entire span of expected groundwater compositions likely to be encountered under oxidising and reducing conditions. The speciation of particular redox-sensitive radionuclides is assessed on an individual basis using the groundwater compositions established by hydrogeological/hydrogeochemical modelling as a basis. Uncertainty distributions for radionuclide-specific K_d values are provided that include both experimental uncertainty and uncertainties regarding the geochemical environment of the rock. For further discussion of parameter values in SR-Site, the reader is referred to the SR-Site Data report /SKB 2010b/ and /Crawford 2010/.

Periglacial and glacial climate domains

The same approach as outlined above for the period of temperate conditions is used for the periglacial and glacial climate domains. K_d values are chosen to represent the relevant geochemical conditions characterising these climate domains.

Earthquakes

Not directly relevant for radionuclide speciation/sorption and therefore neglected.

5.4.8 Uncertainties

Since sorption is a collective term for a number of different processes, it can be claimed that the conceptual understanding varies. The use of the simplification implied by the use of a constant K_d is conceptually and practically attractive, although the validity of this approach can be questioned under certain specific conditions when the prerequisites of the concept (temporally invariable groundwater composition, linearity, reversibility and equilibrium) are not strictly fulfilled. The prerequisites in terms of linearity and equilibrium are generally met for the conditions that apply in the safety assessment, even if competition for sorption sites by major ions may imply non-linearity for some elements. Although groundwater compositions cannot realistically be expected to be static over very long timescales, K_d values are chosen to cautiously overpredict radiological risk where this uncertainty does exist. Thus, the validity of the concept does not in itself entail an uncertainty factor, given the purpose of the safety assessment and provided conditional K_d values are chosen in such a way that retardation is not overestimated.

Sorption modelling based upon site-specific data is used to inform the selection of K_d values for ion exchanging radionuclides. Sorption by way of surface complexation can theoretically be described with mechanistic modelling approaches. These models are general and based upon well-founded theoretical concepts, although they require internally consistent and robust thermodynamic data sets for the sorbing substances and minerals involved in the sorption process. Although great advances have been made in recent years with regard to thermodynamic modelling of safety assessment relevant radionuclides on single minerals and simplified mineral assemblages /NEA 2001, 2005/, the state of the art is deemed insufficiently mature for application within safety assessment modelling for granitic rock.

Uncertainties in mechanistic understanding

There are still a number of outstanding issues concerning interpretation of experimental laboratory data that need to be considered in greater detail before concluding that the compiled K_d values are, indeed, cautious in a performance assessment framework. The formal handling of these uncertainties typically results in expanded ranges of statistical uncertainty which may not be fully representative of the systematic variability of the underlying process with regard to mechanistic dependencies on physicochemical conditions.

Many effects related to the use of crushed rock, effects of contact time, and effects of water composition are not well understood at present. Apart from these issues related to macroscopic data representativity, there is still considerable uncertainty concerning specific mechanisms underpinning sorption processes owing to a lack of data (i.e. internally consistent thermodynamic data for mechanistic modelling, characterisation of mineral phases dominating sorption processes, and spectroscopic confirmation of postulated sorption mechanisms). As a direct consequence of this, there is still considerable uncertainty concerning how best to extrapolate sorption properties derived from laboratory experiments conducted on crushed material to apply to intact rock under *in situ* stress conditions and possibly differing groundwater compositions. It is further noted that even measurements on whole rock pieces in the laboratory may be biased due to mechanical damage effects and possibly non-representative groundwater compositions.

Model simplification uncertainties in SR-Site

The representation of sorption using a conditional K_d approach implies some particular uncertainties in addition to the data interpretation issues outlined above. It should be noted that these forward modelling uncertainties would exist even with perfect knowledge of the mechanistic dependency of the conditional K_d value on physicochemical conditions. These uncertainties are related to the conceptualisation of the reactive transport process itself in safety assessment codes and ideally should be considered as a separate issue to that of sorption data interpretation. It is difficult to completely disassociate these issues, however, since consideration of the subsequent modelling simplifications, by necessity also guides the selection of appropriate K_d data in the first place. Acknowledging this, the K_d values are chosen cautiously with regard to the dynamics of the particular scenarios being modelled and thus do not provide a true representation of the transport mechanisms as they actually occur. Also, the fact that immobilisation processes such as precipitation/dissolution and solid solution formation (co-precipitation) and subsequent remobilisation if chemical conditions change are not included implies that realism is lost.

Input data and data uncertainties in SR-Site

The input data are discussed in detail in the SR-Site Data report /SKB 2010b/ and in the supporting report /Crawford 2010/. The data compilation in /Crawford 2010/ is based on the SDM-Site transport properties evaluation and other pertinent data including recent investigations reported in the open literature and previous data collections /e.g. Crawford et al. 2006, Carbol and Engkvist 1997/. However, the final uncertainty assessment and choice of parameter values for the calculations within SR-Site is made directly in the Data report /SKB 2010b/.

5.4.9 Adequacy of references supporting the handling in SR-Site

The primary reference supporting the selection of data and assignment of uncertainty is /Crawford 2010/. This is an SKB report that has undergone documented factual review. It, in turn, contains reviews and compilations of relevant literature data and supporting analyses reflecting the state of the art.

5.5 Reactions groundwater/rock matrix

5.5.1 Overview/general description

Stagnant groundwater will eventually approach a chemical equilibrium by reactions with the different minerals in the bedrock. Most reactions between water and minerals are, however, so slow that complete equilibrium will never be reached, even if the flux of the water in the bedrock is very slow. If there is a considerable groundwater flow, advection of solutes in the groundwater will promote the dissolution of minerals by removing the reaction products. In the rock matrix, the dissolution products first have to diffuse towards a flowing fracture. Therefore, alteration and larger porosity of the rock minerals is expected at short distances from the fracture surface /Drake et al. 2008, Sandström et al. 2008a/.

The groundwater's many reactions with the rock matrix are of importance for the chemical evolution of the groundwater in general. However, only some of these are of importance for the chemical evolution of the repository in a million-year perspective.

Ever since the rocks were formed nearly two billion years (2 Ga) ago, chemical reactions have affected the rock and its fracture system. During rock formation, water was released that contained residual products, such as chloride, sodium and calcium, that did not fit into the crystal lattice. This water is called magmatic or juvenile water, e.g. /Jackson 1997/. Remnants of this water are preferentially hosted in fluid inclusions and usually contain large quantities of dissolved salts /Waber and Smellie 2008/. Metamorphism or other major tectonothermal events may later significantly have altered the composition of this water.

If the salinity of the water exceeds 10%, i.e. 100 g/L TDS, it is called brine /Frape and Fritz 1987/. Such water is stagnant due to its high density, which increases with time as more salt is leached out of the rock matrix.

The chemical reactions that take place in the groundwater-mineral system have widely varying reaction rates. It is thereby possible to some extent to use known reaction rates to assess the residence time of the groundwater in the rock. The degree of equilibration gives a rough idea of the residence time. Reaction rates for different kinds of reactions have been compiled by /Bruno 1997/. The fastest are metal hydrolysis reactions, with half-lives ranging from microseconds to tenths of seconds. After that follows complexation between metals and organic ligands, with half-lives of hundredths of a second to minutes, whereas fulvic and humic binding reactions proceed about ten times slower. Redox reactions with an electron transfer take from tens of minutes to several years, whereas redox reactions that require changes in molecular structure have half-lives of several to thousands of years.

Reactions that include solid phases (minerals) are generally much slower than reactions that take place in the aqueous phase. Exceptions are ion-exchange reactions, which proceed just as quickly as reactions in the aqueous phase. Dissolving hematite in water takes tens to tens of thousands of years, and dissolution of aluminium silicate takes tens of thousands to millions of years. However, there are reactions between solid phases and water that are considerable faster, e.g. dissolution and precipitation of calcite, which have half-lives of seconds to days.

However, the reaction rate is also strongly dependent on the chemical environment where the reaction occurs. Precipitation of iron(oxy)hydroxide takes from picoseconds up to tens of years, depending on the pH, redox conditions and iron concentrations in the groundwater.

At very high pH, which can occur in contact with concrete, the reaction rates for dissolution of silicate minerals in granitic bedrock are associated with a timescale of months or years. The silicate minerals are dissolved as a consequence of hydrolysis reactions, after which secondary reaction products are precipitated. Valuable knowledge concerning this reaction has been obtained from the hyperalkaline sources in Maqarin in Jordan /Smellie 1998/. Not very much is known about the reaction rate, but it is assumed that the reaction can reduce pH to 10–11 and that it is an extremely thin layer of minerals that reacts. At high pH, the secondary phases consist of calcium silicate hydrates (CSH), which are common in concrete. Zeolites form at lower pH.

Very saline groundwaters (brines) are encountered where drilling has been done to great depths. The depth at which they are encountered varies widely from a few hundred metres to several km. This shows how deep the superficial circulation cells have reached at some time since the brine was formed, which is often millions of years ago. The absence of brine does not necessarily mean that recent circulation of surface waters has occurred, but it does show that water exchange has occurred at this depth at some time since the rocks were formed.

Brines can also be formed by the dissolution of evaporites (salts deriving from an ancient dried-up sea) by infiltrating groundwater. In general, brines of evaporitic origin can be considered to be common in sedimentary rocks, whereas leaching is the probable source of brines in crystalline bedrock (unless they have been overlain by thick sediments which may also have contributed some brine component). In both cases, the occurrence is a clear indication that the water is stagnant.

The effect of the various aforementioned reactions between water and minerals is also evident in the rock. Since the rock was formed, conversion of primary minerals to secondary (clay) minerals has proceeded episodically. This has also affected the rock's porosity and its thermal properties. The effects have been greatest under so-called hydrothermal conditions, when hot aggressive water has passed through the flow paths in the rock, preferentially the major fracture zones. Hydrothermal conditions (> 150°C) at repository depth have, in general, not occurred in the Fennoscandian shield since the Precambrian (i.e. the last 570 million years) /Drake et al. 2009a, Sandström et al. 2009/. During hydrothermal events, primary minerals in the rock adjacent to fractures have been altered into secondary minerals (e.g. albite, chlorite, epidote, hematite), material has been dissolved resulting in increased porosity in the wall rock and dissolution of older fracture-filling minerals and large quantities of fracture-filling minerals have been deposited in the fracture systems /Sandström et al. 2008a, Drake and Tullborg 2009a/. Afterwards, these fracture systems often have been subjected to reactivation on several different occasions, so that the water's previous flow paths in the rock are difficult to trace, even in the large, highly transmissive fracture zones.

During the late Palaeozoic (c. 400 to 250 million years ago), the overlaying sedimentary cover increased the temperature at the present erosion level to 50–150°C in large parts of the Fennoscandian Shield during a period of at least hundred million years /Larson et al. 1999/. Leaching of these sediments led to formation of saline waters which subsequently migrated downward and precipitated fracture minerals like calcite (with very saline fluid inclusions), pyrite and gypsum in the bedrock fractures /Drake and Tullborg 2009b, Sandström and Tullborg 2009/. Even though the water that passed through the rock at that time has disappeared, it can still influence the groundwater through dissolution of phases along the fractures.

In saline groundwater as well, an increasing degree of chemical equilibration is an indication that the water is stagnant. How such waters will evolve in the future is a more difficult question.

The minerals in the rock have a varying tendency to be altered or dissolved in groundwater. The same reactions probably take place on a microscale in the rock matrix and on a macroscale in water-bearing fracture zones. The difference is mainly that the water in the matrix is stagnant and transport of reactants and reaction products takes place mainly by diffusion /Waber et al. 2009a/. There is no sharp borderline between water-bearing fractures and the rock matrix.

Studies of porewater chemistry in the URL (Underground Research Laboratory) in Canada show that the rock matrix at depth contains very saline water compared with lower salinities in water-bearing fractures /Gascoyne et al. 1996/. In contrast, at Äspö there is a similarity between matrix porewater and water in water-bearing fractures in the near-vicinity, essentially both being brackish /Smellie et al. 2003/. More recent studies at Laxemar by /Waber et al. 2009a/ show porewater with about the same salinity as the fracture groundwater down to about 400 m depth, where the fracture frequency and transmissivity is high. A change to porewaters that are more saline than the fracture groundwater occurs below this depth down to at least 500 m, where the bedrock is characterised by a low frequency of water-bearing fractures. Toward greater depths, the porewater has a lower salinity than the fracture groundwater.

Corresponding studies at Forsmark by /Waber et al. 2009b/ show that in the bedrock of the target volume (below the gently dipping deformation zones ZFMA2 and ZFMF1) down to about 640 m, the porewater and fracture groundwater are in a transient state with a more dilute porewater in the rock matrix than in the fracture groundwater. The porewater has preserved an older chemical signature, probably pre-dating the last glaciation. In the upper part of this bedrock down to a depth of about 150 m, this old signature is modified by a younger brackish marine (i.e. Littorina-type) water and possibly glacial water. Below a depth of about 640 m, the porewater becomes increasingly saline and similar to the highly saline groundwater in Laxemar. No fracture groundwater data exists from these depths at Forsmark.

Influence on pH; The rock's minerals are of importance for the groundwater pH. There is a direct influence that is dependent on the interaction between the water and readily soluble minerals such as calcite, and an indirect influence that is controlled by slow weathering, the chemistry of the water and microbial conditions. There is a clear tendency for the pH to increase with depth, i.e. with the residence time, for non-saline waters, with extreme values of up to pH of about 10. The pH values for saline waters lie within a narrower range and seldom exceed 8.5. However, pH values below 7 and as low as 5.2 do occur at great depth (more than 1,000 m) in extremely saline Canadian brines /Frape and Fritz 1987/. For several granitic rock types, it has been shown that hydrogen ions at mineral surfaces can be replaced by cations in the water releasing H^+. The pH thereby becomes lower in saline than in non-saline groundwaters /Toulhoat et al. 1992/.

Influence on redox conditions; The bedrock content of reducing substances such as sulphide, divalent iron and manganese is vital for maintaining reducing conditions in the groundwater. The capacity to resist an attack by oxidising substances – such as oxygen trapped in the repository on closure, or oxygen-rich water that infiltrates down on melting of an ice sheet – exists in the minerals, preferentially in the iron(II)-bearing minerals biotite, chlorite, clay minerals and pyrite. The redox level, or Eh, and the kinetics of the reactions are determined by the dominant redox pairs in solution along with the variety and quantity of microbes.

5.5.2 Dependencies between process and geosphere variables

Table 5-4 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.5.7.

Table 5-4. Direct dependencies between the process "Reactions groundwater/rock matrix" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. By changes in reaction types and rates.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.	Yes. By producing or consuming heat.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.
		Glacial	Influence neglected; little significance compared with other influences.		Glacial	Influence neglected; little significance compared with other influences.
Groundwater flow	No. But indirectly by keeping groundwater concentrations at a "constant" level.	–	–	No.	–	–
Groundwater pressure	Yes. But the effect of pressure on reaction rates is negligible.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.	No.	–	–
		Glacial	Influence neglected; little significance compared with other influences.			

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Gas phase flow	No. But indirectly a gas phase flowing in a fracture will dissolve into the pore waters of the rock matrix and diffuse in the pore water. Dissolved reactive gases such as O_2 and CO_2 will react with the rock minerals.	–	–	No. But indirectly via the porewater contents of dissolved reactive gases such as O_2 and CO_2, which subsequently may come out of solution.	–	–
Repository geometry	No. But indirectly via changes in flow through hydraulically active fracture zones that become short-circuited and subsequent changes in water composition. This effect is minor.	–	–	No.	–	–
Fracture geometry	Yes. Porosity affects mineral surfaces accessible to reactions.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.	Yes. Weathering reaction may increase or decrease the porosity of the rock matrix.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.
		Glacial	Porosity included in the modelling of the consumption of O_2 in infiltrating glacial meltwaters.		Glacial	Influence neglected; little expected impact.
Rock stresses	No. But indirectly by affecting matrix porosity.	–	–	No. But indirectly by changing porosity.	–	–
Matrix minerals	Yes.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.	Yes.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.
		Glacial	Included in the modelling of the consumption in the rock matrix of O_2 infiltrating in glacial melt waters.		Glacial	Included in the modelling of the consumption in the rock matrix of O_2 infiltrating in glacial melt waters.
Fracture minerals	No. But indirectly by hindering matrix diffusion.	–	–	No. But indirectly through porewater chemistry and matrix diffusion, but this is a very slow process.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Groundwater composition	Yes.	Excavation/ operation Temperate Periglacial	The effects on dissolution-precipitation reactions in the rock matrix induced by the propagation of changes in chemical composition of groundwaters in fractures are not considered in SR-Site. Observations of drillcores indicate that this influence is negligible.	Yes.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.
		Glacial	Included in the modelling of the consumption in the rock matrix of O_2 infiltrating in glacial melt waters.		Glacial	Included in the modelling of the consumption in the rock matrix of O_2 infiltrating in glacial melt waters.
Gas composition	No. But indirectly via gas phase dissolution and diffusion in the pore water in the rock matrix. Dissolved reactive gases such as O_2 and CO_2 will react with the rock minerals.	–	–	No. But indirectly by affecting the porewater contents of dissolved reactive gases such as O_2 and CO_2.	–	–
Structural and stray materials	No. But indirectly by affecting pH, sulphide etc of groundwater, see Section 5.8	–	–	No.	–	–
Saturation	Yes. Reactions between rock and porewater can only take place in the saturated portions of the rock matrix.	Excavation/ operation Temperate Periglacial	Process neglected; little expected impact compared with the effects of reactions with fracture-filling minerals.	Yes. But negligible production of gaseous products by porewater-rock reactions	All	Disregarded: Too small amounts of gaseous species involved in water-rock reactions.
		Glacial	Saturated conditions assumed.			

5.5.3 Boundary conditions

There are no particular conditions at the geosphere boundaries for the reactions between groundwater and rock matrix.

5.5.4 Model studies/experimental studies

With the aid of thermodynamic calculation tools, it is possible to determine which mineral alterations can be expected under different conditions. The accuracy of the data and knowledge of the reactions is sufficient. Detailed knowledge and data on the reaction kinetics is less satisfactory, which makes it difficult to get an idea of what time spans need to be postulated to achieve equilibrium.

5.5.5 Natural analogues/observations in nature

There are many examples from nature which underline the water-rock reaction sequence from the introduction of meteoric water at shallow depths, to the evolution of deeper groundwaters of increasing salinity, to finally the formation and existence of deep-seated brines. Evolution of the general sequence of water-rock reactions in crystalline rock environments has been addressed by natural analogue studies at Palmottu, Finland /Pitkänen et al. 2002, Négrel et al. 2003/ and from the various site investigations in Sweden and Finland /Blyth et al. 2000, Laaksoharju et al. 2008b, 2009a, Drake and Tullborg 2009a, Sandström and Tullborg 2009/. Geochemistry of crystalline basement brines has been documented from Canada, Russia and Fennoscandia /e.g. Lahermo and Lampén 1987, Sie and Frape 2002, Négrel and Casanova 2005, Négrel et al. 2004/. The oscillating behaviour of the brine/less saline interface during glacial events has been reported from the Sellafield site, UK /Bath et al. 2000/.

5.5.6 Time perspective

Very saline water, brine, will remain unchanged during the short (geologically speaking) period of time appropriate to a post-closure safety assessment of disposal of spent nuclear fuel. The fact that brines still exist is attributable to their stability in time caused by their higher density. This is also true of the primary minerals in the rock. The conditions that prevail today will remain relevant during the entire life of the repository, although there is a possibility that the brines may migrate in the bedrock during glacial events.

Chemical reactions that influence the composition of the water occur in a timeframe of thousands to hundreds of thousands of years. Producing a water type with extremely high salinity (brine) requires much longer periods. The prevailing chemical groundwater composition is the result of many different ongoing reactions and mixing of different waters /Laaksoharju et al. 2008a/. Because the reactions have been going on for a long time, they have reached a static situation where the effects of different reactions balance each other. The composition can thereby be regarded as static, i.e. it will remain as it is unless changes in the flow conditions cause changes in the mixing proportions between different water types.

5.5.7 Handling in the safety assessment SR-Site

This process is not deemed to cause appreciable changes in groundwater composition or matrix porosity for the whole time period during which the function of the repository must be considered.

Excavation/operation period, temperate- and periglacial climate domains

During the excavation/operation phase, aerated waters could be expected to flow in fractures in the vicinity of the tunnels, or in the excavation damaged zone, but chemical reactions are expected to take place only at the surfaces of fractures and not in the rock matrix. The evidence from drillcores is that the weathering process within the rock matrix in the candidate rock volumes of Laxemar and Forsmark is negligible. Therefore, mineral dissolution and transformation of the rock matrix are not modelled in SR-Site, except for periods of glacial conditions, see below.

Glacial climate domain

Beneath a warm-based ice sheet, water could possibly penetrate down to repository depth. It is expected that these melt waters initially will contain dissolved O_2. The consumption of dissolved oxygen is evaluated by calculation of the reactions during transport down into the rock. Reactions that consume O_2 in the groundwater include dissolution of iron(II) minerals (biotite, chlorite or pyrite), present both as fracture infillings and within the rock matrix.

Earthquakes

Fracturing of the rock due to earthquakes is not likely to have a significant effect on the hydrogeochemistry at repository depths unless fracturing causes significant changes in the flow conditions, resulting in mixing of different groundwaters. Mixing of groundwaters could lead to dissolution and/or precipitation processes between water and rock matrix. However, it is inferred that bedrock movements at repository depth mainly would occur by reactivation of existing fractures and not in the intact rock, see Section 4.3.

5.5.8 Uncertainties

Uncertainties in mechanistic understanding

Many different mineral alteration reactions influence the evolution of the water chemistry, and in extreme cases, the formation of brines. The end result of these reactions is generally well known. The uncertainty relates to the kinetics of the reactions, where it is known that many reactions are extremely slow. It is, therefore, also unreliable to regard the water/mineral system as if it were in equilibrium and thereby capable of being described solely using thermodynamic data. Due to the inertia in the system, i.e. its slow kinetics, only small changes caused by dissolution and precipitation in the rock matrix can be expected over the geologically short time span relevant in disposal of spent nuclear fuel.

Model simplification uncertainties in SR-Site

In the oxygen intrusion models, oxygen is assumed to react with ferrous iron comprised in the rock matrix minerals (see further next subsection). Thus, organic material and other reducing species in the matrix are pessimistically neglected.

The heterogeneity of the rock matrix is simplified to an equivalent homogeneous porous medium. Hydrothermally altered layers are commonly found in the rock matrix adjacent to fractures. The observed increased porosity in these layers is neglected in the models.

The hydraulic properties in the rock below the margin of an ice sheet are expected to change dramatically during its passage. Flow rates are expected to increase and the flow pattern may change so that e.g. discharge flow-paths become recharge paths. These transient effects during ice margin passage are not captured in the oxygen intrusion models. Instead different glacial scenarios and ice-front locations are modelled as stationary “snap-shots” of hydraulic properties.

Input data and data uncertainties in SR-Site

Regarding the reducing capacity, the ferrous iron in the matrix is assumed to be present in biotite. Ferrous iron in e.g. pyrite is thus modelled as if it were comprised in biotite. This is a pessimistic simplification since dissolution of biotite is a slow process compared with other ferrous minerals.

Based on theoretical constraints, the oxidation capacity in intruding glacial melt water is assumed to be five times larger than in water in contact with the atmosphere. This high value is generally not measured in glacial melt waters, but is supported by /Raynauld and Lebel 1979/ who found that glaciers in Greenland contained 2.9 to 4.5 times more air occluded in the ice than what would be dissolved in water at 0°C.

The uncertainty in dissolution rates of biotite is to a large extent related to the specific reactive surface of the mineral grains. In the oxygen intrusion models, the pore space between mineral grains is assumed to be connected so that all grains are available through diffusion in the pores. The initial reactive surface is based on experimental estimations of the geometrical surfaces of the grains, and corrected for surface roughness. Based on observations of completely oxidised ferrous mineral grains, all ferrous iron is assumed to be available for reaction. Uncertainties regarding available reactive surfaces and specific reaction rates are handled in the models by studying the effects of parameter variations.

5.5.9 Adequacy of references supporting the handling in SR-Site

All supporting references in this section are either peer reviewed scientific papers or SKB reports that have undergone a documented factual and quality review.

5.6 Dissolution/precipitation of fracture-filling minerals

5.6.1 Overview/general description

Minerals on fracture surfaces can dissolve in the groundwater and, conversely, solutes in the groundwater can precipitate on fracture surfaces. These processes are in general controlled by the advection of solutes in the groundwater. Products from the dissolution reactions are either removed, and this promotes further dissolution, or new reactants are brought in contact with the solid phases to drive the precipitation process. In addition to advection/mixing, other factors that may induce dissolution or precipitation of fracture infillings are changes in temperature, pressure, pH, redox conditions and salt exclusion induced by freezing /e.g. Puigdomenech 2001, Sandström et al. 2009/.

Under steady-state conditions, these processes are as a rule very slow. In the case of transient processes, e.g. infiltration (inflow) of acid or oxygenated water in the bedrock, the capacity of the fracture-filling minerals to buffer (counteract) chemical changes is important. In the case of radionuclide transport, the interaction between dissolved radionuclides and fracture surfaces is important.

Reactions between water and fracture-filling minerals give rise to conversion (alteration) of the mineral phases. At the surface, this phenomenon is called chemical weathering, and the mineral phases formed consist e.g. of different kinds of clay minerals and iron(oxy)hydroxides. Many bedrock fractures show complex evolution with repeated reactivation and precipitation of new fracture minerals. The sequence of different events of fracture mineral precipitation can be revealed by detailed investigations /Sandström et al. 2008b, Drake and Tullborg 2009a/. However, in water-bearing fractures, recent alteration often makes it difficult to determine when and under what conditions precipitation has taken place. Most fracture-filling minerals at Forsmark and Laxemar have originated under hydrothermal conditions (temperatures above 150°C) during the Precambrian (>540 Ma) or from brine-type fluids at temperatures between 60 and 190°C during the Palaeozoic (>250 Ma) /Drake et al. 2009a, Sandström et al. 2009/. Subsequently, they have been subjected to alteration on several different occasions.

Precipitated minerals, formed by mixing of waters of different compositions, are also present on individual fracture surfaces. Precipitated fracture minerals, such as calcite, gypsum, pyrite, fluorite, zeolites and iron oxides, make it possible to draw qualitative conclusions concerning the water chemistry that prevailed when the minerals were formed /Drake and Tullborg 2009a, Sandström and Tullborg 2009/. By contrast, the opposite reactions, dissolution of fracture-filling minerals, are difficult to identify and quantify. Rapid transport of carbon dioxide-rich water can, for example, dissolve calcite in a flow path relatively rapidly, causing precipitation of calcite on the fracture surfaces when subsequently mixing with other types of water. Calcite minerals in the same fracture have been investigated at different depths to provide information on the dissolution rate and thereby the groundwater flux /Landström and Tullborg 1995/.

Influence on fracture geometry; Due to the relatively rapid dissolution and precipitation reaction with calcite, the flow paths in the rock will be changed if the chemistry of the infiltrating groundwater is changed. Open fractures will be healed and previously healed fractures may be opened due to changes in water chemistry. Only in the event of major climate changes could this effect possibly be significant. The presence of Palaeozoic and even Precambrian calcite at both Forsmark and Laxemar indicates that major events of calcite dissolution are not common /Drake and Tullborg 2009a, Sandström and Tullborg 2009/. Significant dissolution of calcite due to infiltrating surface water has been showed at Laxemar, but is restricted to fractures in the uppermost 25–35 metres /Drake et al. 2009b/.

Geochemical modelling of the mineral precipitation potential in the excavation damaged zone (EDZ) in the rock around the deposition tunnel shows that precipitation of calcite and ferric oxyhydroxides is thermodynamically feasible during repository construction and after repository closure. Preliminary results indicate that the time required to completely seal the few tens of centimetres of EDZ around the tunnel is between several hundreds to more than a million years /Acero et al. 2009/.

Influence on sodium and calcium concentrations; Meteoric recharging water that contains calcium gains sodium with depth, whereas infiltrating seawater loses sodium in exchange for calcium. The reason is ion exchange, which takes place in clay minerals along with weathering and precipitation reactions. As a result of these reactions, the water, regardless of whether it is fresh or saline, will have particular concentrations and proportions of sodium and calcium. Very dilute groundwaters are unusual at great depths, and the calcium concentration generally exceeds 10 mg/L at repository depth. At both Forsmark and Laxemar, the calcium concentration at 500 m depth is of the order of 500 mg/L /SKB 2008a, 2009a/. This is important, since calcium destabilises colloidal particles at a concentration in excess of about 40 mg/L (see Section 5.9).

Influence on magnesium and potassium concentrations; The cations magnesium and potassium are common in groundwater, but their concentration is kept down by uptake in smectite clays and precipitation reactions. This is clearly evident at sites where seawater has infiltrated the rock and the concentrations have fallen from originally high marine Mg/Cl and K/Cl ratios to lower ratios in the fracture groundwater /Laaksoharju et al. 2008b, 2009a/.

Influence on pH; The pH of the groundwater is normally in the range 6.5–9.5. Of greatest importance for the pH in the infiltrating groundwater are reactions between carbon dioxide dissolved in the water and calcite in the rock's fracture system and overburden. The carbonate system quickly reaches a state of equilibrium and determines the water's pH, which will then be around 8.5 /Stumm and Morgan 1981/. The total carbonate concentration at repository depth varies from <10 to about 150 mg/L at Forsmark /Laaksoharju et al. 2008b/ and from about 10 to 200 mg/L at Laxemar /Laaksoharju et al. 2009a/.

With increasing depth, the carbonate concentration usually decreases and the salinity increases. Saline groundwaters that have been isolated for a long time generally have a lower pH than non-saline stagnant waters. The reason is that hydrogen ions located in the mineral layers can be replaced by cations in the water so that more protons come out into solution and the pH thereby becomes lower than in non-saline groundwaters /Toulhoat et al. 1992/.

The carbonate content of non-saline deep waters also declines with increasing residence time as an effect of increasing pH. The increasing pH is a result of feldspar weathering, which releases calcium which, by precipitation of calcite, further lowers the carbonate concentration. However, the pH-buffering capacity which exists in the carbonate system in the groundwater, and which determines the pH, is small in comparison with the buffering capacity in the minerals. The amount of calcite that coats the fracture surfaces is of greater importance for buffering against acidification than the carbonates in the aqueous phase. Feldspars also have a large capacity to buffer against acidification. A quantitative example of the capacity of feldspar was given in a study in Poços de Caldas, Brazil, where a superficial groundwater with a pH of 3 was changed to 6–7 by reaction with feldspar /Nordstrom et al. 1992, Chapman et al. 1993/.

Calcite is a useful indicator of inflow of recently infiltrated groundwater. In Laxemar, where carbon dioxide-rich groundwater has infiltrated the bedrock, calcite dissolution can be seen to have occurred down to a depth of about 35 m /Drake et al. 2009b/. Calcite occurs as a fracture-filling mineral in a large proportion of the water-bearing fractures (at Laxemar in about 70–90% of the fractures /Drake and Tullborg 2009b/ and at Forsmark in around 60–80% /Byegård et al. 2008/). For water-conducting fractures and fractures in the vicinity of water-conducting fractures, where the averaged fracture mineral thickness and visible coverage could be quantitatively estimated, arithmetic means for calcite in Laxemar are 0.25 mm and 22% /Löfgren and Sidborn 2010a/, respectively, and in Forsmark 0.11 mm and 18%, respectively /Löfgren and Sidborn 2010b/. The calcite minerals thereby constitute an effective buffer against infiltrating acid groundwater. Various analyses have been performed for the purpose of describing how acidification will affect the groundwater composition at repository level /Wersin et al. 1994/. The conclusion is that the capacity of the minerals in the rock is sufficient to buffer against any acidification that can reasonably be expected.

Influence on redox conditions; Under the undisturbed conditions that prevail before the repository is built and that are expected to be reinstated some time after closure, it can be assumed that conditions are reducing and that the Eh of the groundwater is controlled by iron and sulphide minerals in the rock and is sufficiently low that uranium, neptunium, plutonium and perhaps technetium in solution occur in reduced, poorly soluble forms. The Eh is linked to the pH and varies within the range –100 to –400 mV for pH values in the range 7–9.

The redox buffering capacity will lie in the available iron(II) and sulphide minerals in the fractures, which will react rapidly, and in the very large amount of reducing minerals in the rock matrix itself, which will be accessed by diffusion. Iron(II)-bearing chlorite, clay minerals and pyrite are the most abundant fracture minerals with reducing capacity at Forsmark and Laxemar /Sandström et al. 2008b, Drake and Tullborg 2009b/. The rock matrix makes up, by far, the largest potential reducing capacity, which will become active when there are no reducing minerals in the fracture or when originally present minerals have been exhausted. Numerous experiments have been conducted to explore both the reaction kinetics /Malmström et al. 1995/ and the capacity /Pirhonen and Pitkänen 1991/ of iron-bearing minerals.

Co-precipitation of radionuclides; Precipitation and dissolution reactions may affect radionuclide transport. Small amounts of radionuclides may be entrained in e.g. the calcite lattice in conjunction with the precipitation of some mineral phases. This process is called co-precipitation. Trace substances that occur in the groundwaters can be modelled in terms of co-precipitation, and it is possible that the concentrations in groundwater of some radionuclides could be controlled by this process /Bruno et al. 1996/.

5.6.2 Dependencies between process and geosphere variables

Table 5-5 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.6.7.

Table 5-5. Direct dependencies between the process "Dissolution/precipitation of fracture-filling minerals" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. Reaction rates and solubilities are temperature dependent.	Excavation/ operation Temperate	Influence neglected; little significance compared with other influences.	Yes. Reactions can produce or consume heat.	All	Neglected; the effect on temperature is negligible.
		Periglacial	Process neglected; of little significance to water composition and matrix porosity.			
		Glacial	Influence neglected; little significance compared with other influences.			
Groundwater flow	No. But indirectly through advection of solutes, necessary to the precipitation and dissolution reactions.	–	–	No. But indirectly by changing fracture geometry and matrix porosity.	–	–
Groundwater pressure	Yes. Changes in pressure may change solubility.	All	Neglected; effect on reaction rates and solubilities is negligible.	No.	–	–
Gas phase flow	No. But indirectly by providing nutrients for microbially mediated reactions that change the stability of fracture filling minerals.	–	–	No. But indirectly by changes in fracture geometry (aperture).	–	–
Repository geometry	No. But indirectly via changes in flow through hydraulically active fracture zones that become short-circuited and subsequent changes in water composition.	–	–	No.	–	–
Fracture geometry	No. But indirectly via changes in the flow that could induce changes in groundwater chemistry/reactions	–	–	Yes. Geometry might be changed by the sealing or opening of some fractures.	Excavation/ operation Temperate period	Generic modelling that indicates that this influence is negligible.
					Periglacial Glacial	Process neglected; little significance.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Rock stresses	No. But indirectly if previously sealed fractures become reopened, followed by healing.	–	–	No.	–	–
Matrix minerals	No. But indirectly by the release of ionic species that may be incorporated in fracture precipitating phases.	–	–	No.	–	–
Fracture minerals	Yes.	All	Common fracture minerals (calcite, silica, etc.) selected for generic equilibrium calculations. Influence of Fe(II) fracture filling minerals on O_2 consumption evaluated.	Yes.	All	Common fracture minerals (calcite, silica, etc.) selected for generic equilibrium calculations. Influence of Fe(II) fracture filling minerals on O_2 consumption evaluated.
Groundwater composition	Yes.	All	Generic modelling of precipitation-dissolution of minerals.	Yes.	All	Generic modelling of precipitation-dissolution of minerals.
Gas composition	No. But indirectly, e.g. methane may be a source of nutrients for microbially mediated reactions that could induce mineral precipitation or dissolution.	–	–	No. But indirectly, e.g. precipitation of calcite will influence the amount of CO_2 in a possible gas phase: $CO_2 + H_2O + Ca^{2+} = CaCO_3(s) + 2H^+$.		
Structural and stray materials	No. But indirectly since, e.g. iron from corrosion may result in the precipitation of iron oxides/hydroxides.	–	See Section 5.8.	No.	–	–
Saturation	Yes. Fracture-filling minerals will only precipitate in the saturated parts of the rock.	All	Influence neglected; little significance.	No.	–	–

5.6.3 Boundary conditions

There are no particular conditions at the geosphere boundaries for the dissolution and/or precipitation of fracture-filling minerals. The relevant conditions in order to treat stability of fracture minerals quantitatively are the groundwater concentrations in the different parts of the system being modelled.

5.6.4 Model studies/experimental studies

See Overview/general description.

5.6.5 Natural analogues/observations in nature

In the Poços de Caldas project, the effects of co-precipitation as a retention process were evaluated for analogues to radionuclides /Bruno et al. 1996/. Since then, several of the international and domestic analogue and site characterisation studies have addressed the mechanisms of radionuclide (and other trace element) retention in fractures from different types of host rocks representing different hydrogeological/hydrogeochemical environments /Tullborg et al. 1999, Kaija et al. 2000, Smellie 2002, Byegård et al. 2008/.

Fracture minerals can also be used to verify the present groundwater chemistry and to yield information about past groundwater conditions (palaeohydrogeology). The minerals used in such studies are mostly calcites, as this is a common fracture mineral that can form under various conditions. By analysing its stable isotope composition (O and C), Sr isotope ratio and its trace element contents, information about formation conditions can be obtained /Bath et al. 2000, Tullborg 2003, Drake and Tullborg 2009b, Sandström and Tullborg 2009/.

Analyses of fracture calcites have also been used to support the presence of former microbial activity in the fractures /Pedersen et al. 1997, Tullborg et al. 1999, Drake and Tullborg 2009b, Sandström and Tullborg 2009/.

Uranium contents and uranium decay series analyses on groundwater and fracture minerals can indicate redox conditions over a time span of 1 Ma. Results from Äspö and Laxemar indicate changes from oxidising to reducing conditions within the upper 50 m of the bedrock /Tullborg et al. 2003, Drake and Tullborg 2009a/. This is also supported by the distribution of the redox-sensitive fracture minerals goethite and pyrite and by anomalous contents of the redox-sensitive element Ce (cerium) in the fracture coatings. At Forsmark, mobilisation as well as redeposition of uranium in the upper 150 metres of the bedrock is indicated. This is ascribed to the transition from near-surface oxidising conditions to more stable reducing conditions at depth /Sandström et al. 2008b/.

5.6.6 Time perspective

Dissolution and precipitation reactions in fracture systems are fast in comparison with the weathering of the primary minerals. These reactions are therefore of importance in a repository perspective. It is necessary to take into account the consequence for fracture minerals of keeping the repository open, and the fact that it takes some time before the initial undisturbed conditions are restored.

5.6.7 Handling in the safety assessment SR-Site

For the influence of co-precipitation on radionuclide transport, see Sections 5.4 and 6.1.

Excavation/operation period, temperate-, periglacial- and glacial climate domain

With knowledge of the hydrochemical conditions at the sites of interest, advection and mixing processes are evaluated and the equilibrium situation is calculated for the most common fracture-filling minerals, such as calcite, gypsum, siderite, fluorite, barite, and pyrite. The computer software PHREEQC is used for these calculations /Parkhurst and Appelo 1999/. The effects of precipitation-dissolution of grout are studied through generic calculations /Grandia et al. 2010/, see Section 5.8.

Beneath a glacial ice sheet, oxygenated water could possibly penetrate down to repository depth. Oxygen reactions with fracture-filling minerals are considered in analyses of oxygen penetration to repository depth (see also Section 5.5).

Earthquakes

Fracturing of the rock due to earthquakes is not likely to have a significant effect on the hydrogeochemistry at repository depths unless fracturing causes significant changes in the water flow, and subsequent mixing of different groundwaters, which is unlikely. Mixing of groundwaters would, if such substantial fracturing should occur, lead to dissolution or precipitation of fracture minerals along water-conductive fractures. Such events are, however, neglected in SR-Site.

5.6.8 Uncertainties

Uncertainties in mechanistic understanding

The dissolution and precipitation of minerals are simple processes that may be well described and modelled either at equilibrium or as slow rate-controlled processes. The difficulty in practice is to establish the nature of the solid phase being formed or dissolved. For example, co-precipitation reactions are known for certain solid phases and trace substances. There is a large uncertainty as to whether these reactions apply generally.

Model simplification uncertainties in SR-Site

Only precipitation and dissolution of solid phases that are known to have fast kinetics at low temperatures are used in modelling, e.g. carbonates, amorphous silica, Fe(III) oxides and oxyhydroxides.

Salt exclusion caused by freezing might induce precipitation of some minerals, such as mirabilite ($Na_2SO_4{\cdot}10H_2O$), inside fractures. This might have consequences on fracture conductivity and groundwater flow, but this effect will be minor compared with the solidification of water into ice. However, changes in fracture properties, such as porosity, are not considered in SR-Site.

Input data and data uncertainties in SR-Site

The thermodynamic properties control mineral solubilities, and they are well known for fracture-coating minerals that have formed at low temperatures, i.e. those that have been precipitated due to supersaturation in groundwater.

However, there is some difficulty in establishing these properties for the much larger quantity of fracture-filling minerals that have arisen under hydrothermal conditions. There is also an uncertainty regarding the origin of certain iron(III) oxides, where it is of importance whether they have formed under hydrothermal conditions or through low-temperature oxidation by oxygenated groundwater. The variability, co-existence and spatial distribution of different minerals are poorly understood. The effects of these data uncertainties are discussed in the reports for the corresponding modelling exercises /Byegård et al. 2008, Crawford 2008, Sidborn et al. 2010/.

5.6.9 Adequacy of references supporting the handling in SR-Site

All supporting references in this section are either peer-reviewed scientific papers or SKB reports that have undergone a documented factual and quality review.

5.7 Microbial processes

5.7.1 Overview/general description

Microbial processes comprise the decomposition and the production of organic molecules with different electron donors, energy sources and electron acceptors. Organic carbon, including methane, and reduced inorganic molecules, including hydrogen, are possible electron donors and energy sources for microbial processes in the geosphere. During the microbial oxidation of these energy sources, microorganisms preferentially reduce electron acceptors in a particular order as shown in Figure 5-2. First oxygen, and thereafter nitrate, manganese, iron, sulphate, sulphur and carbon dioxide are reduced. Simultaneously, fermentative processes supply the metabolising microorganisms with, for example, hydrogen and short-chain organic acids such as acetate. As the solubility of oxygen in water is relatively low, and because oxygen is the preferred electron acceptor of many bacteria that utilise organic compounds in shallow groundwater, anaerobic environments and processes usually dominate at depth in the subterranean environment. The reduction of microbial electron acceptors may significantly alter the following geosphere variables: groundwater composition and fracture minerals. Dissolved nitrate is reduced to N_2 (see Section 5.10), solid manganese and iron oxides in fracture minerals are reduced to dissolved species, and the sulphur in sulphate is reduced to sulphide. In addition, the metabolic processes of some autotrophic microorganisms produce organic carbon, such as acetate, from the inorganic species carbon dioxide and hydrogen, whereas other microorganisms produce methane from these species; all microbial processes generally lower the redox potential, Eh.

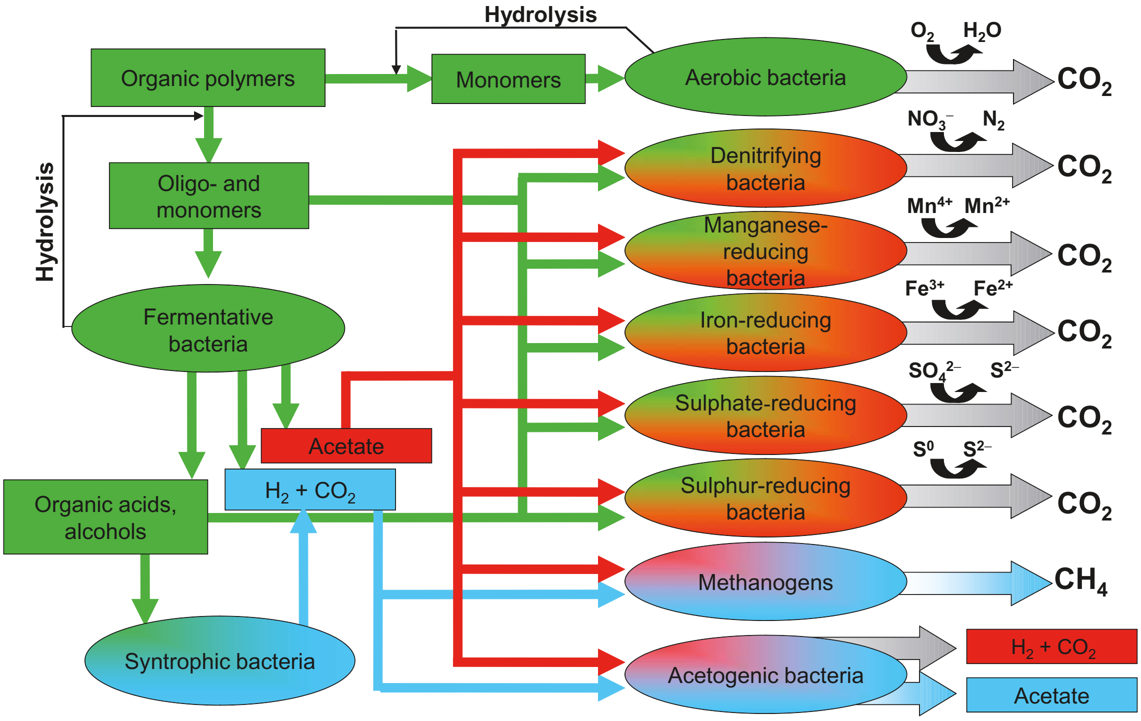

***Figure 5-2.** Possible pathways for the flow of carbon in the geosphere environment. Organic carbon (green and red) is respired to carbon dioxide with oxygen (black/grey), if present, or else fermentation (green) and anaerobic respiration (black/grey) occurs with an array of different electron acceptors. Autotrophic processes (blue) generate methane and acetate from carbon dioxide and hydrogen.*

Growth

Growth is defined as a microbial process where coordinated increase in the mass of essential cell components leads to cell division and an increase in the number of cells. The geosphere variable 'structural and stray material' can be influenced by this microbial process because during growth, microorganisms oxidise various organic and inorganic energy sources (Table 5-6). The harvested energy is used to synthesise new cell components such as cell walls, proteins, fat, carbohydrates and nucleic acids. The microorganisms produce organic molecules that can be expelled to the environment for purposes such as chelating agents for trace elements needed for growth and polymers enhancing attachment and biofilm formation. During growth, many microorganisms excrete waste products such as alcohols, organic acids and carbon dioxide.

Table 5-6. The most common energy and electron donors and electron acceptors in microbial metabolism. The respective atom that donates or accepts one or several electrons is underlined.

Organic energy sources and electron donors		Inorganic energy sources and electron donors		Electron acceptors	
Reduced	**Oxidised**	**Reduced**	**Oxidised**	**Oxidised**	**Reduced**
Carbohydrates	$\underline{C}O_2$			$\underline{O}_2$	$H_2\underline{O}$
Amino acids	$\underline{C}O_2$	$\underline{N}H_4^+$	$\underline{N}O_3$	$\underline{N}O_3$	$\underline{N}_2$
Organic acids	$\underline{C}O_2$	$\underline{Mn}^{2+}$	$\underline{Mn}^{4+}$	$\underline{Mn}^{4+}$	$\underline{Mn}^{2+}$
Fat	$\underline{C}O_2$	$\underline{Fe}^{2+}$	$\underline{Fe}^{3+}$	$\underline{Fe}^{3+}$	$\underline{Fe}^{2+}$
$\underline{C}H_4$	$\underline{C}O_2$	$H_2\underline{S}$	$\underline{S}O_4^{2-}$	$\underline{S}O_4^{2-}$	$H_2\underline{S}$
		$H_2\underline{S}$	$\underline{S}^0$	$\underline{S}^0$	$H_2\underline{S}$
		$\underline{C}O$	$\underline{C}O_2$	$\underline{U}O_2^{2+}$	$\underline{U}^{4+}$
		$\underline{H}_2$	$\underline{H}_2O$	$\underline{C}O_2$	$\underline{C}H_4$

Respiration

A general microbial process is respiration, which must proceed in all active microorganisms, except for those running a fermentative metabolism. Respiration is a membrane-bound process where electrons from metabolic, dissimilatory, oxidative processes are expelled from the cell via the reduction of different electron acceptors. The electron donors to the metabolic processes can be either organic compounds or inorganic, reduced molecules (Table 5-6). Respiration mainly influences the following geosphere variables: groundwater composition, gas composition and fracture minerals. This is because the process of respiration changes the state of oxidation, and commonly also the state of aggregation, of the respective electron acceptor. Representative microorganisms for all types of microbial respiration processes discussed below, and depicted in Table 5-6 have been found in Fennoscandian groundwater down to repository depths /Hallbeck and Pedersen 2008a, Pedersen et al. 2008/. The diversity and numbers of microorganisms was investigated in detail in the site investigations of Laxemar /Hallbeck and Pedersen 2008b/ and Forsmark /Hallbeck and Pedersen 2008c/.

Oxygen. Oxygen is the preferred electron acceptor by many microorganisms, because the free energy change available in oxidation of electron and energy donors is larger when oxygen is used compared with all other metabolic electron acceptors. Oxygen is a species that is reduced to water. This process of reduction thereby influences the gas composition in the geosphere and removes oxygen from any system where aerobic respiration (with oxygen) is possible, resulting in a decreasing Eh. A full-scale atmospheric oxygen intrusion experiment into a 70 m deep vertical fracture zone at the Äspö HRL (Hard Rock Laboratory), Sweden, showed that microbial oxygen reduction may be of considerable importance in granitic environments /Banwart et al. 1996/. Monod modelling of microbial kinetics of respiratory oxygen reduction has been applied on data from field and laboratory experiments /Kotelnikova 2002, Molinero et al. 2004, Yang et al. 2008/.The most important conclusion was that microbial oxygen reduction processes play a substantial role in granitic environments, by contributing to the removal of oxygen that infiltrates into the ground. This microbial process is most relevant in the shallow groundwater zone above a repository, as judged from data obtained in Olkiluoto, Finland /Pedersen et al. 2008/. Oxygen respiration in shallow groundwater, consequently, explains why almost all deep groundwater systems are anaerobic. Microbial oxygen reduction will be active during the excavation/operation and temperate time periods. It is presently not well established to what extent this microbial process will be active during permafrost and glaciations. It can be assumed that some oxygen reduction will be ongoing with methane from crustal processes during cold periods.

Nitrate. In oxygen depleted (anaerobic) systems, nitrate is the preferred electron acceptor in microbial respiration. Nitrate is commonly present as a dissolved ion. The reduction of nitrogen in nitrate can result in different products depending on the environmental conditions for this respiratory microbial process. Commonly, the end product is N_2; when the carbon and energy source is plentiful relative to nitrate, e.g. in manure, the process tends to end with ammonium. However, such conditions seldom occur in deep groundwater but may be relevant if large amounts of organic structural stray material occur in the repository. This process consequently alters the state of aggregation of the electron acceptor from a dissolved ion to a gaseous species in most cases and thereby influences the geosphere variables gas composition and groundwater composition. The main sustainable source of nitrate to groundwater should be from surface ecosystems, in particular from soil fertilisers. As concluded above, oxygen is rapidly removed by microbial respiration processes in shallow, infiltrating groundwater. When oxygen is used up, nitrate will be reduced. Most deep groundwater systems are, consequently, depleted not only in oxygen but also in nitrate when electron donors are abundant. Microbial nitrate reduction will be active during temperate time periods and possibly also during the excavation/operation period. It is presently not well known to what extent this process will be active during permafrost and glaciations.

Iron and manganese. Solids containing iron(III) and manganese(IV), such as some oxides and fracture minerals, can serve as electron acceptors in microbial respiratory processes that degrade organic carbon compounds /Nealson et al. 1988, Lovley 1991/. In this process, the state of aggregation is changed from solid to dissolved, and the geosphere variables ‘fracture minerals’ and ‘groundwater composition’ are influenced. The microorganisms can dissolve solid fracture metal oxides either by direct contact or by remotely operating chelating agents and nanowires /Reguera et al. 2005/. This microbial process will be active during the excavation/operation and temperate time periods. It is presently not well known to what extent this process will be active during permafrost and glaciations.

Uranium; Microbial processes have the potential to affect the fate of uranium in a variety of environmental settings /Anderson and Lovley 2000/. The reduction of U(VI) to U(IV) is a well-known process where U(VI) acts as electron acceptor analogous to what has been described above for iron and manganese /Lovley et al. 1991/. The state of aggregation of uranium is then changed from dissolved to solid (uranium(IV) oxide is quite insoluble), and the geosphere variables 'fracture minerals' and 'groundwater composition' are influenced.

Sulphate, sulphur; In systems depleted in oxygen and nitrate, sulphate commonly becomes the preferred electron acceptor (over CO_2), if available, for microbial respiration. Sulphate is a dissolved species that is reduced to the gaseous species hydrogen sulphide, which is readily soluble in water with a significant dependence on pH, as it easily dissociates into HS^- at $pH > 7$. The reductant can be hydrogen, organic carbon or methane /Boetius et al. 2000/. In this process, the state of aggregation is changed from dissolved ion (i.e. sulphate) to a gaseous species (hydrogen sulphide) and possibly also to solids in the form of insoluble metal sulphides. The geosphere variables 'fracture minerals', 'gas composition' and 'groundwater composition' are therefore influenced. A major effect from sulphate reduction was found on redox potential during the site investigations, as revealed by the correlations between numbers of sulphate reducing bacteria (SRB) and measured redox potential /Hallbeck and Pedersen 2008b, 2008c/. Several types of microorganisms can reduce elemental sulphur to sulphide, but as elemental sulphur is rare in granitic groundwater environments, it is not further treated here. The biological nature of sulphate reduction in natural and engineered systems has been well investigated /Muyzer and Stams 2008/ and the process is ubiquitous in most anaerobic aquatic systems with temperatures below 110°C. The corrosive nature of sulphide for metals makes this process very important to understand and quantify. Microbial sulphate reduction will be active in anaerobic environments during the excavation/operation and temperate time periods. It is presently not well known to what extent this process will be active during permafrost and glaciations.

Methylation and alkylation

Some metals and metalloids can be converted by a variety of microorganisms to their volatile methyl derivates. Such methylation of metals is the substitution of one hydrogen atom in methane (CH_4) by a metal atom. Alkylation of metals with alkanes can also occur. Metals and metalloids known to be subject to biomethylation include Hg, Se, Te, As, Sn, Pb and Cd. In addition, aqueous solutions of methyl iodide may react with metals causing them to dissolve /Thayer et al. 1987/. It has been predicted that Pt, Pd, Au and Tl can also be transformed in this way. This conversion of metals to methylated forms can be mediated by microbes under both aerobic and anaerobic conditions. In aerobic environments, this activity appears to be principally (but not exclusively) associated with fungi. Under anaerobic conditions, methylation can be carried out by a variety of bacteria (e.g. clostridia, sulphate-reducing bacteria, methanogens).

Microbial methylation and alkylation of radionuclides can be regarded as a special case of radionuclide mobilisation. Microorganisms perform several different methylation reactions in their metabolism /Francis 1990/. Radionuclides could not only be mobilised, but also their bioavailability and radiotoxicity could change, as the process can change an aqueous soluble metal cation into a metalorganic molecule soluble in organic solvents (such as fat) /Lloyd and Macaskie 2002, Macaskie and Lloyd 2002/.

Anabolic processes

Anabolism is a term used for a number of processes by which microorganisms synthesise the vast array of chemical substances of which they are composed. Autotrophic microorganisms can synthesise all organic cell components such as proteins, fat, carbohydrates and nucleic acids, needed for growth with inorganic energy and electron donors and carbon dioxide as the carbon source (Table 5-6).

Acetogenesis. Autotrophic acetogens produce acetate from hydrogen and carbon dioxide during growth /Wood and Ljungdahl 1991/. They produce more acetate than needed for anabolic processes and acetate is, therefore, expelled to the environment (Figure 5-2). This process influences mainly gas and groundwater composition.

Methanogenesis. Autotrophic methanogens produce methane from hydrogen and carbon dioxide during growth /Oremland 1988/. The methane is expelled to the environment (Figure 5-2). This process influences mainly gas composition.

Extracellular metabolites, enzymes, complexing agents. Many microorganisms synthesise organic components that are expelled to the outside of the cell. These compounds can be enzymes for the degradation of polymers and complexing agents targeted at trace elements but also affecting radionuclides /Lloyd and Macaskie 2002/. The complexing agents mainly interact with the geosphere processes of 'transport of radionuclides in the water phase' and 'speciation and sorption' (see Section 5.4). Other microorganisms excrete acids under fermentative conditions which is a process that may interact with degradation of grout /Diercks et al. 1991/ (see Section 5.8). Microorganisms produce various kinds of chelating compounds to increase the bioavailability of essential elements needed for metabolism, such as low molecular mass organic acids (LMMOAs) and siderophores. These ligands are not always highly specific, and several of them will also mobilise other elements such as non-essential metals and radionuclides /Johnsson et al. 2006, Essén et al. 2007/. Siderophores produced by deep groundwater bacteria cultured in the laboratory have been demonstrated to bind uranium /Moll et al. 2008a/ and curium /Moll et al. 2008b/. The potential for uranium mobilisation from shale by groundwater bacteria has been established /Kalinowski et al. 2004, 2006/. The potential for the mobilisation of radionuclides from deep granitic repository environments by bacterially produced ligands is unknown, and it warrants further exploration. However, all information available so far indicates that the potential for mobilisation is probably negligible, since natural levels often are in the nanomolar range e.g. /Rue and Bruland 1995, Macrellis et al. 2001, Holmström et al. 2004/.

Biofilm formation

Many microorganisms attach and grow on surfaces of all types in aquatic systems. The resulting cover of microorganisms on a surface is commonly termed a biofilm. Formation of biofilms on surfaces in groundwater systems has been observed by /Ekendahl and Pedersen 1994, Ekendahl et al. 1994/. Microbial biofilms have been demonstrated to interact with the process of speciation and sorption of metal ions /Anderson et al. 2006a/. It was found that biofilms on granitic rock decreased the sorption of some radionuclides /Anderson et al. 2006b/. Groundwater with radionuclides that emerges on the surface will commonly encounter mats with biological iron oxides /Ghiorse and Ehrlich 1992/. The mix of microorganisms and iron hydroxides in these mats has a strong retardation effect on trace elements /Anderson and Pedersen 2003/ and radionuclides may, therefore, be efficiently immobilised. Because of the constant growth of bacteria, the biofilms will be renewed continuously as long as the right conditions are met. Even if the biofilm is gone, the mineralisation of iron hydroxides will remain.

Since biofilms can be expected to partially cover fracture surfaces they may have an influence on diffusive uptake to the rock matrix and sorption properties of the flow-exposed surfaces. However, scoping calculations made in /Crawford 2008/ and /Crawford and Sidborn 2009/ indicate that the overall impact on the retardation of radionuclide transport should, for all practical purposes, be negligible for the ranges of hydrodynamic transport resistances (F-factors) typically associated with safety assessment conditions.

It is well known that microorganisms can attach to minerals and dissolve them, e.g. volcanic glass /Staudigel et al. 2008/. In addition, it has been observed that microorganisms are involved with precipitation of fracture fillings /Pedersen et al. 1997/ and clays /Ehrlich 1999, Tuck et al. 2006/. The biofilm formation process consequently influences dissolution/precipitation of fracture-filling materials, and in fact all "low"-temperature (below 100°C) fracture minerals present in the vicinity of the repository have been precipitated in the presence of microbes and their biofilms.

Predation

Microorganisms are under constant predation pressure from viruses, so called phages. Phages may control the numbers of microorganisms in active ecosystems. This has been demonstrated for sulphate-reducing bacteria in deep groundwater /Eydal et al. 2009/. The phages commonly outnumber the microorganisms about 10 times /Kyle et al. 2008/. The process of predation influences all microbial processes due to its nature as population control. In other words, phages may limit the rates of microbial processes. Viruses that attack microorganisms commonly occur in numbers up to 10^9 particles per litre of groundwater. Their size range typically is 20 – 500 nm which places them in the size range of colloids. Consequently, viruses contribute to the number of colloids in groundwater, see also Section 5.9.1. Viruses consist of proteins that may be strong sorbents for radionuclides, just as microorganisms sorb radionuclides /Pedersen and Albinsson 1991/. Mobilisation of radionuclides by phages is a plausible process not yet investigated, although this process is similar to colloid-enhanced radionuclide transport.

5.7.2 Dependencies between process and geosphere variables

Table 5-7 shows how microbial processes are influenced by and influence all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.7.7.

Table 5-7. Direct dependencies between microbial processes and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. The rate of microbial processes generally increases with increasing temperature.	All.	Influence neglected; little significance compared with other influences.	No.	–	–
Groundwater flow	Yes. Biofilm formation processes are stimulated by increasing flow rate	Excavation/ operation Temperate Periglacial Glacial	Influence neglected, since biofilms in excavated areas can be removed before closure. Influence neglected due to low flow rates Influence neglected; presumably low levels of nutrients.	Yes. Through biofilm formation. Indirectly; microbial activity may over time contribute to the generation of fracture minerals that eventually seal a fracture.	All	Influence neglected. All groundwater data obtained at the site already include the presence of biofilms. Effects from changes in biofilm thickness are deemed negligible.
Groundwater pressure	No. But indirectly via the influence of pressure on groundwater and gas composition.	–	–	No.	–	–
Gas phase flow	No.	–	–	No.	–	–
Repository geometry	No. But indirectly through changes in groundwater flow.	–	–	No.	–	–
Fracture geometry	Yes. Cavities smaller than 0.2 μm in diameter are not accessible to microbes.	All.	Neglected. This influence has negligible effect on the overall microbial activities in the rock volume around the repository	No. But indirectly fracture sealing might result from formation of fracture-filling minerals resulting from microbial activity.	–	–
Rock stresses	No.	–	–	No.	–	–
Matrix minerals	No.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture minerals	Yes. Several microbial respiration processes depend on solid electron donors present in some minerals.	All.	Process not handled in detail; variations in the amounts of fracture minerals have a low impact on the overall microbial processes.	Yes. Biological weathering of specific mineral components; Formation and dissolution of metals sulphides and calcite; Stable isotope fractionation of fracture minerals; coverage with biofilms.	All.	Process not handled in detail. The production-consumption of fracture minerals by microbial processes have a low impact on the overall amounts of minerals.
Groundwater composition	Yes. Groundwater provides nutrients for microbial metabolism.	All.	Process not handled in detail; sulphate reduction assumed to proceed to completion.	Yes. Microbial processes will influence concentrations of groundwater components, dissolved gases, Eh and to some extent pH.	All.	Process not handled in detail; sulphate-sulphide equilibrium calculations assuming microbial mediation. Sulphide contribution from possible CH_4+H_2 accounted for.
Gas composition	No. But indirectly if a gas phase containing components such as oxygen, hydrogen or methane were to occur and dissolve in groundwater.	–	–	No. But indirectly microbial metabolic products may, e.g. produce gaseous components such as CO_2 and this could affect the composition of a gas phase if present.	–	–
Structural and stray materials	Yes. Organic carbon in materials and hydrogen from corrosion will support and increase microbial activity.	All.	Process not handled in detail; calculations of sulphide production assuming microbial reduction with structural and stray materials.	Yes. Microbial processes will oxidise organic carbon in materials and hydrogen from corrosion, thereby influencing construction material and corrosive processes.	All.	The degradation of iron, steel and organic stray materials evaluated for different time periods.
Saturation	No.	–	–	No.	–	–

Temperature in bedrock. The rate of the biochemical reactions generated by microbial activities generally increases with increasing temperature. The degradation of structural and stray material will be more rapid during the high temperature phase, compared with later phases. This variable will increase the rate of microbial processes during the warm phase, relative to the later periods with ambient temperatures and cold conditions during permafrost and glacial periods.

Groundwater flow. The potential for biofilm formation is positively correlated to flow rate /Characklis and Marshall 1990, Pedersen 1982/. During excavation, biofilms will tend to form on the tunnel walls and floor where groundwater is draining into the tunnels. Biofilms may also contribute to sealing of fractures. After closure, flow rates will be very slow and the biofilm formation process will be limited. During glaciation periods, groundwater flow at repository depths might increase under the passage of the ice-front.

Groundwater pressure. Microorganisms consist mainly of water and do not have gas-filled spaces. Most microorganisms are not sensitive to hydrostatic pressure. However, indirect effects may be present due to the influence of pressure on groundwater and gas composition.

Gas phase flow. There are no relevant direct effects from the flow of a gas phase on microbial processes. However, indirectly, the flow and dissolution of gaseous components into an aqueous solution will change the water composition and as a consequence it will most probably affect the microbial processes in the water phase.

Repository geometry. There are no relevant direct effects of repository geometry on microbial processes, but indirectly such effects could occur through alteration of groundwater flow.

Fracture geometry. The smallest size a microorganism can take is a sphere of about 0.2 µm in diameter. This excludes microbial processes from all cavities smaller than this diameter, including cavities that may be larger, but with access restricted to pores smaller than 0.2 µm diameter. However, nanowires and chelating agents produced by microorganisms might be present in the pore space of the rock matrix.

Rock stresses. There are no relevant direct effects of rock stresses on microbial processes.

Matrix minerals. The fracture geometry of the rock matrix is generally below the smallest size a microbe can take, 0.2 µm, and microbial processes are, therefore, not possible in the rock matrix. Indirectly, microbial processes may influence matrix minerals through diffusion into the matrix of microbial metabolic products that may affect weathering reactions. This process is expected to be of negligible importance.

Fracture minerals. Ferric iron, manganese oxides and hexavalent uranium in fracture minerals will support respiratory microbial processes with electron acceptors, thereby influencing this geosphere variable. In the case of oxygen intrusion, sulphides can be used as electron donor and a source of energy by sulphur-oxidising bacteria. Microbial processes may influence fracture minerals in several other ways. Biological weathering, as discussed for biofilm processes above, is possible. Several microbial products will influence fracture minerals, such as the generation of metal sulphides via sulphate reduction to sulphide, and the dissolution/formation of calcite due to microbial production of carbon dioxide during growth on organic compounds. The microbial stable isotope fractionation of iron, sulphur and carbon will influence the isotope signatures of fracture minerals. Finally, formation and coverage of biofilms on mineral surfaces may alter the radionuclide retention properties of minerals.

Groundwater composition. The concentrations of metabolites such as carbon sources, electron donors and electron acceptors in groundwater will influence which of the microbial processes will take place. The active processes will run for as long as the respective metabolites for different processes are available. The rate of the microbial process will be controlled mainly by temperature and phage predation. Microbial processes will influence groundwater composition significantly by their reduction of electron donors during respiration, which will change the states of oxidation and aggregation of important groundwater components. Removal of oxygen, nitrate and hydrogen from the groundwater composition and production of N_2, sulphide, ferrous iron, manganese(II), carbon dioxide and methane will have a profound influence on groundwater composition. Microbial processes will also influence redox and to some extent pH. In particular, redox conditions depend of the production of ferrous iron, hydrogen consumption and the involvement of sulphide in microbial respiration processes. A special case is the anaerobic oxidation of methane with sulphate to carbon dioxide and sulphide, which has been documented to take place in sediments. Whether this occurs in the geosphere or not is not known. The microbial populations reach a steady state with the surrounding environment. However, it is still an open system where new components may be introduced.

Gas phase composition. Gas phase composition is not expected to have a direct effect on microbial processes. However, an indirect effect is possible if components of the gas phase dissolve and affect the groundwater composition.

Structural and stray materials. Many construction materials, such as grout, contain organic additions that can be used by many microorganisms. Microbial processes, therefore, may also influence the construction material by removal and degradation of important components. The anaerobic corrosion of iron in wire mesh and rock bolts will generate hydrogen that is a preferred source of electrons and energy for many microorganisms. Hydrogen will increase microbial growth and hence the rate of microbial processes that result in acetate and sulphide.

Saturation. There are no relevant direct effects of saturation on microbial processes.

5.7.3 Boundary conditions

Relevant conditions in order to treat the microbial processes quantitatively are the concentrations of nutrients and of electron acceptors and donors in the different parts of the system being modelled. These are, in turn, dependent on the flux of these components across the boundaries, i.e. the boundary conditions for the processes advection and gas flow. In this respect there are three important, indirect boundary conditions for microbial processes in the geosphere.

The input of organic material and oxygen from the surface biosphere will influence the rate and extent of microbial processes in the geosphere. In cases where the input of organic carbon exceeds the amount of oxygen needed for degradation in intruding groundwater, microbial processes will continue under anaerobic conditions.

A second boundary is the interface between the geosphere and repository tunnels and deposition holes with backfill, buffer and construction material. The flux of organic carbon and hydrogen from these areas will determine rate and extent of microbial processes in the geosphere close to the repository system. This boundary is also important to understand when canister corrosion is considered. Microbial processes produce sulphide in the geosphere, and the copper canister acts as a sink for sulphide. The concentration of sulphide at the buffer/geosphere boundary will determine the diffusion rate of sulphide and the concomitant copper corrosion rate /Pedersen 2010/.

The third boundary is between the geosphere and deep, subsurface gas-generating areas /Apps and van de Kamp 1993/. The flux of hydrogen and methane from mantle processes into the geosphere will determine the possible rates of microbial processes that utilise hydrogen and methane.

5.7.4 Model studies/experimental studies

A large and diverse array of investigations and experiments has been conducted to increase the understanding of microbial processes in deep groundwater and repositories /Pedersen 2001, 2002/. Sampling procedures have been developed and thoroughly tested as have underground facilities for model studies /Nielsen et al. 2006, Hallbeck and Pedersen 2008a/ The first important parameter to analyse in repository environments is biomass. Three different methods have been developed and found to correlate. Microscopic counts and biochemical analysis of adenosine-tri-phosphate (ATP) agreed well /Eydal and Pedersen 2007/. The determination of cultivable microorganisms and ATP also agreed well when analysed /Pedersen et al. 2008/. All types of microorganisms indicated in Figure 5-2 have been found via cultivation /Hallbeck and Pedersen 2008a/, including fungi /Ekendahl et al. 2003, Reitner et al. 2005/. Recently, the influence of viruses on microbial processes has been identified as an important factor to include in model studies. In particular, they seem to have an important mitigation effect on sulphide production by sulphate-reducing bacteria /Kyle et al. 2008, Eydal et al. 2009/.

Microbial biofilms were found to significantly influence the sorption of radionuclides on glass and rock surfaces /Anderson et al. 2006a, b/. In addition, it has been demonstrated that microbial iron-oxidising biofilms are strong sorbents for trace elements /Anderson and Pedersen 2003, Anderson et al. 2006c/. Microorganisms from deep groundwater produce complexing agents that mobilise radionuclides /Johnsson et al. 2006, Essén et al. 2007/. Such complexing agents have a strong influence on radionuclide mobility. They can mobilise uranium /Kalinowski et al. 2004, 2006/ and strongly bind curium /Moll et al. 2008a/ and uranium /Moll et al. 2008b/. Interactions between SRB and curium have also been identified /Moll et al. 2004/. Finally, it has been found that microorganisms can sorb radionuclides on their cell surfaces /Pedersen and Albinsson 1991/, thereby facilitating mobilisation.

Microbial consumption of oxygen in a repository after backfilling has been modelled /Yang et al. 2007/. It was found that presence of oxygen-reducing microorganisms decreased the time to consume all oxygen dramatically from several hundreds of years to a few weeks. A model to analyse microbial and geochemical reactive transport in porous media was successfully applied on field experiment data from an underground hard rock environment /Yang et al. 2007/. Microbial metabolic processes have been included in transport models /Molinero et al. 2004/ of a redox zone experiment /Banwart et al. 1994/. The modelling supported previous conclusions on the importance of microbial processes in the reduction of oxygen with organic carbon /Banwart et al. 1996/.

5.7.5 Natural analogues/observations in nature

The Palmottu U-Th deposit in Finland and the Bangombé natural nuclear reactor in Gabon are both considered natural analogues for subsurface radioactive waste disposal. The microbial population naturally present in groundwater may affect the redox conditions, and hence, the radionuclide solubility and migration. Therefore, groundwater samples from the two sites were investigated for microbial populations /Pedersen et al. 1996, Crozier et al. 1999, Haveman and Pedersen 2002/. The results suggest that microorganisms can be expected to play a role in stabilising radioactive waste disposed of in the subsurface by lowering the redox potential and immobilising radionuclides.

The alkaline springs of Maqarin have been thoroughly investigated for microbial activity /Pedersen et al. 2004/. The results demonstrated that microorganisms from the hyper-alkaline springs of Maqarin can grow and be metabolically active under aerobic and anaerobic hyperalkaline conditions. However, the growth and activity found were not vigorous. Rather, slow growth to low numbers and a generally low metabolic activity *in situ* were found. This suggests that microbial activity will be low during the hyper-alkaline phase of cementitious parts of the repository.

5.7.6 Time perspective

Extensive microbial activity can be expected in conjunction with the operation and closure of the repository, when mixing of oxidising and reducing waters occurs. During this initial period, the largest amounts of organic materials will be found at or near the repository. These organics may be grout-cement additives, hydraulic oil spillage, pollen introduced with ventilation air, etc. and they may be used as nutrients for microbial processes. Grout, shotcrete and concrete elements will create zones of increased groundwater pH. This could reduce microbial activity. After closure, microbial activity will continue at a high rate, correlated with temperature. After the repository has cooled down, microbial process rates will be slower than during the high-temperature phase when the access to organic material from structural and stray material is high and microbial growth rates significant.

Changes in groundwater flow and chemistry induced by climate-related changes, e.g. by permafrost, ice sheets and shoreline displacements, will affect the microbial activities in the geosphere. During glaciations, the input of organic matter from the surface with recharge waters is expected to be substantially reduced, and microbial activities will be limited to processes using dissolved methane and hydrogen from large depths. In periods where sea water covers the repository site, larger amounts of sulphate and organic matter would be expected to be present in the recharge waters, facilitating the microbial reduction of iron(III) and sulphate.

5.7.7 Handling in the safety assessment SR-Site

Excavation/operation period

During excavation and operation, a large pool of organic material will be introduced as structural and stray material. In addition, corrosive material will generate hydrogen that is a preferred source of energy and electrons for many microorganisms. An inventory of material that can be utilised by microbial processes after closure has identified three main pools /Hallbeck 2010/. The largest pool of organic material in a repository is the organic material in bentonite in the buffer and tunnel backfill. The second largest pool will be the biofilms formed on the rock surfaces. During the excavation/operation period, bacteria and iron hydroxide will accumulate when reducing groundwater meets atmospheric oxygen in tunnels.

If this precipitation proceeds for a long time, significant amounts of biofilm will be deposited on the tunnel walls and may remain there after closure, unless cleaned out. An estimate is made of how large these quantities could be, and what consequences this process may have /Hallbeck 2010/. The third largest pool is the material that can be produced by microorganisms with hydrogen from anaerobic corrosion of iron in steel, as an energy source. Mass balance calculations are coupled with microbial process descriptions and rates and integrated with solute transport and hydrochemical equilibria calculations to show how different kinds of residual organic materials and corroding metals remaining in the repository will be degraded by microbial processes during the excavation/operation period. It is assumed that all organic matter and hydrogen from corrosion will be able to serve as energy and carbon sources for microorganisms.

Temperate climate domain

During the initial warm period, an increased microbial activity will be expected until all residual, degradable organic matter and hydrogen from corroding iron has been consumed and the repository has cooled to ambient temperature. Mass balance calculations are coupled with microbial process descriptions and rates and integrated with solute transport and hydrochemical equilibria calculations. This is to show how different kinds of residual organic materials and corroding metals remaining in the repository will be degraded by microbial processes during the temperate period. It is assumed that all organic matter and hydrogen from corrosion will be able to serve as energy and carbon sources for microorganisms. Subsequent microbial activity will be controlled by the supply of hydrogen and methane. In the long run, all oxygen and some of the iron(III), sulphate and carbon dioxide will be reduced. The availability of hydrogen and methane will be a primary control on microbial activity in the long term.

Periglacial- and glacial climate domains

Until recently, it was believed that glacial systems were abiotic /Gibbs and Kump 1994/. Periods of glaciation would then present a special case. During such events, the input of organic carbon with recharging groundwater is expected to be low, because during glaciation, photosynthetic production of organic carbon will cease. However, an increasing number of studies now verify the opposite, and a recent review by /Hodson et al. 2008/ thoroughly summarises current knowledge of organisms and biological processes in glacial environments. Studies of glaciers and ice-sheets around the world have demonstrated that microorganisms and other organisms thrive not only in snow cover and surface ice environments, but that organisms can also be found *in* the ice at various depths and in subglacial environments. The biogeochemistry and ecology of glaciers, ice sheets, and permafrost is still a young scientific niche, and research has been ongoing for only approximately 20 years. The most studied parts of the glacier system are the supra- and subglacial environments. The most important findings from the literature study are that primary production by photosynthesis is ongoing in the snow cover and ice surfaces of glaciers and ice sheets /Hallbeck 2009/. Heterotrophic microorganisms in the supraglacial environment consume organic material and oxygen. Anaerobic environments can be found in the cores of surface ice blocks. The subglacial environment is very active containing several kinds of microorganisms, both aerobic and anaerobic. The oxygen concentration in the subsurface varies depending on whether the surface water has been transported over a long or short residence time. The proglacial environment is also microbially active, containing rivers and lakes filled with glacial meltwater /Hallbeck 2009/. There are microbial populations in these watersheds.

In addition to biological activity in the ice, that may introduce organic carbon and other groundwater components over the ground surface to the geosphere boundary, up-welling methane and hydrogen from deep crustal layers will feed the microbial reduction of oxygen in the infiltrating glacial melt waters. It can be argued that intruding groundwater could flush away methane-containing groundwater and that the oxygen reduction reaction might not occur. However, it is expected that the rock matrix contains methane and other dissolved gases in concentrations similar to those found in groundwater. Consequently, if methane is consumed or flushed out from the fractures of an aquifer, methane will diffuse from the rock matrix into the fractures and the process can continue. As the volume of the rock matrix porosity is larger than the volume of groundwater in the fractures, this process could continue throughout a glaciation cycle, but with reduced intensity to that during temperate conditions.

The consequences of microbial processes under permafrost are not analysed in SR-Site, as the dominating processes under this period, in addition to freezing, are salt exclusion and methane ice formation.

Earthquakes

There are no relevant direct effects of earthquakes on microbial processes.

5.7.8 Uncertainties

Uncertainties in mechanistic understanding

The available knowledge of the effects of different microbial processes on repository performance and the preconditions for their existence is generally good. More quantitative information about concentrations and fluxes of carbon and electron sources, and electron donors is needed and additional knowledge is required about microbial *in situ* process rates.

- Existing qualitative and quantitative models of the influence of microbial processes on groundwater composition, gas composition and fracture minerals need to be refined, and adapted to climatic and other changes that may influence the environmental conditions of a repository.
- Existing qualitative and quantitative models of microbial sulphide production need to be refined, and adapted to climatic and other changes that may influence the environmental conditions of a repository.
- Existing qualitative and quantitative models of microbial oxygen consumption need to be refined, and adapted to climatic and other changes that may influence the environmental conditions of a repository.
- The effect of microbial biofilms and microbial complexing agents on the process of transport of radionuclides needs to be further explored.

Remaining uncertainties in the understanding of microbial processes are such that the effects of microbes on repository performance may be qualitatively assessed, but detailed modelling is still uncertain. However, this will be considered in future safety assessment.

Model simplification uncertainties in SR-Site

Modelling of microbial activities generally makes use of the Monod model. The rates are generally fast, days to weeks, as compared with the time scales of advection combined with matrix diffusion and reactions with rock matrix minerals, which take place on time scales longer than years. The coupling of groundwater flow and multi-component solute transport with hydrochemical and microbial processes is computationally time-consuming and simplifications are required in the modelled geometries and in the number of processes modelled. The results of the modelling are strongly coupled to the microbial processes considered and to the values of the parameters used. The simplifications used, such as the exclusion of matrix diffusion in some models, result in underestimates of the rates of oxygen consumption, since the contribution from other processes and reactants that could diffuse from the rock matrix into the fractures is neglected.

Gases such as H_2 and CH_4 are produced from deep crustal processes /Apps and van de Kamp 1993/ and may be transported to repository level at a rate limited by advection and diffusion processes. Their availability will be decisive for microbial activity in the long term. Consequently, after an expected initial increased effect of microbial activity until all residual organic matter and hydrogen from corrosion processes have been consumed, the subsequent microbial activity at repository depth will be controlled by the supply of hydrogen and methane. In the long run, some of the sulphate will be reduced to sulphide near the buffer or backfill, and this sulphide could diffuse to the canister causing some copper corrosion. In addition, intrusion of sea water during the excavation and operation phases might also induce the reduction of sulphate into sulphide, if methane is present. Microbial reduction of sulphate into sulphide is considered no to be a problem as long as the buffer surrounding the canister remains intact. However, the evaluation of a worst case scenario where the buffer is completely lost is included in the safety assessment.

Input data and data uncertainties in SR-Site

Great variability exists in where and to what extent the different microbial processes occur. However, bacterial reduction of oxygen in the shallow groundwater has been documented /Pedersen et al. 2008/ and should occur widely. Corrosion of iron in the repository, e.g. rock bolts and the iron insert in the canister, generates hydrogen, which, in turn, generates acetate that can be used by microbes to produce sulphide. Some quantitative information about acetate and sulphide production has been obtained under *in situ* laboratory conditions, but the applicability of these numbers is unknown /Hallbeck and Pedersen 2008a/. Another source of uncertainty relates to the quantitative estimation of sensitive parameters associated with microbial kinetics, such as growth rate and half saturation constants in the Monod expressions, metabolic process rates and influences from predation. Such parameters are both microbe dependent and environment dependent. Usually, parameter values are obtained in laboratory conditions by means of physiological (i.e. growth) *in vitro* experiments that cannot be fully representative of repository conditions. Results of current *in situ* microbe investigations, as well as model calibration based on field experimental data could be helpful for the up-scaling of key microbial parameters. Nevertheless, model calculations involving microbial processes, even if they are calibrated against experimental field data, are necessarily of qualitative value. However, quantification of the relevant microbial processes will be considered in future safety assessments.

5.7.9 Adequacy of references supporting the handling in SR-Site

All references supporting the handling of microbial processes have been published as peer-reviewed papers or are SKB reports that have undergone a documented factual review.

5.8 Degradation of grout

5.8.1 Overview/general description

The purpose of grouting is to reduce the permeability of the rock surrounding the repository during the excavation and operation phases. Grout degradation will increase the permeability of grouted volumes at significantly later times than repository closure. The increase in permeability due to cement dissolution is considered in the modelling study supporting SR-Site /Grandia et al. 2010/.

Fracturing of the rock close to the galleries and deposition tunnels may require the use of rock bolts, shotcrete and grouting to: a) reinforce the rock to ensure safe working conditions; b) decrease the hydraulic conductivity (e.g. $< 10^{-12}$ m·s^{-1}) in order to avoid unnecessary lowering of the groundwater table and the consequent up-coning of saline waters; and c) reduce inflow to deposition holes and tunnels to facilitate emplacement of buffer and backfill, and to keep the buffer and backfill intact. These materials are not chemically stable in a deep repository and will eventually decompose and affect the groundwater composition.

Cement grouting is the injection of a cement-water mixture at high flow rate and pressure into the rock voids. The cement-water mixture is transformed into hardened cement paste, with the main binding phases comprising calcium silicate hydrates (C-S-H) and calcium hydroxide (CH). In addition, two other major hydration products are produced from reactions involving the aluminate, aluminoferrite, and calcium sulphate, known as AFt and AFm, which are complex calcium ferri-aluminates.

Hardened cement paste is a porous medium, due to the large water/cement ratio of the original cement grouting. The interstitial solution of a regular Portland-based paste will reach chemical equilibrium with the cement constituents, resulting in a hyperalkaline porewater (pH around 13) with large concentrations of alkaline Na^+, K^+, OH^- and Ca^{2+} ions. In the future Swedish spent fuel repository, it is planned to use a "low pH" cement, consisting of a mixture of Portland-type Ultrafin 16 cement and silica fume, at 1.37:1 weight proportion /SKB 2010j/. The porewater pH in equilibrium with low pH cement constituents is estimated to be around 11 or lower. The contact of this alkaline cement porewater with dilute groundwater (pH lower than 9) creates large concentration gradients that induce diffusive mass transport (of mainly Ca^{2+} and OH^- ions) outwards from the porous cement paste. Renewal of the external groundwater by advection will drive away the cement porewater components and accelerate the diffusion of ions and the degradation of grout. The alkaline cement porewaters will react with fracture filling and rock minerals through a complex set of reactions that finally neutralise the alkalinity and produce calcium silicate hydrates, see for example /Hoch et al. 2004, Wan et al. 2004/.

The durability of cement paste is affected by the decalcification process, since calcium is the main component of cement hydrates. The continuous outwards diffusion of Ca^{2+} alters the original chemical equilibrium, which induces dissolution of calcium compounds as the natural tendency to restore chemical equilibrium. In Portland-based cements, the dissolution of highly soluble calcium hydroxide (portlandite) and Ca-rich C-S-H phases leads to an increase in the porosity of the cement paste, which at the same time enhances the diffusion rate. Low-pH cements have negligible quantities of portlandite and larger amounts of C-S-H phases than regular Portland-based cements. C-S-H solubility is complex due to its amorphous to semicrystalline structure, which used to be described as tobermorite-like structures intermixed with others of jennite-like structure /Taylor 1986/. Successive investigations have shown that C-S-H have a large variability in their composition, nanostructure and morphology /Richardson 2004/. A recent exhaustive review on the microstructure of C-S-H is found in /Richardson 2008/. Perhaps the most relevant features of C-S-H solubility relate to their conditions of formation /Flint and Wells 1934, Roller and Ervin 1940, Taylor 1950, Kalousek 1952, Greenberg and Chang 1965, Fujii and Kondo 1981, Barret et al. 1983, Brown et al. 1984, Grutzeck et al. 1989/. More recent studies /Chen et al. 2004/ suggest that C-S-H solids are present under different metastable phases that are susceptible to transform into (replace) one another in the long term. Despite the very low crystallinity of C-S-H solids, they have been considered for convenience as solid solution series, especially when experimental data need to be modelled (e.g. /Kulik and Kersten 2001, Carey and Lichtner 2007/).

Simultaneously with the dissolution of calcium silicate hydrates, the other mineral phases in the cement assemblage are also involved in the leaching phenomena. AFm dissolution releases $Al(OH)_4^-$ which could induce precipitation of either secondary AFm or Ettringite (in the presence of sulphates), whose large molar volume may close off the porous structure /Lagerblad 2001/. In the case of an external groundwater containing carbon dioxide, precipitation of calcite might be expected, which was found to reduce the degradation rate by sealing the pore network on the exposed surface of cement paste /Pfingsten 2001/. Brucite is also prone to precipitate at the cement-groundwater interface, due to the lower pH environment /Lagerblad 2001/.

The chemical composition of the external groundwater affects the rate of grout degradation. Laboratory experiments have shown that the degradation depth is highly dependent on the carbonate concentration of the external aggressive solution. A recent study /Moranville et al. 2004/ showed that leaching depth decreases by a factor of 5 when the external water is in equilibrium with atmospheric CO_2, due to the sealing produced by calcite precipitation at the cement-water interface. An external groundwater containing dissolved sulphate could also have a large impact on the longevity of concrete material /Höglund 2001/ due to ettringite precipitation. The reason is that ettringite has the ability to bind crystal ("adsorbed") water, resulting in a large molar volume of this mineral phase, which results in cracking and mechanical deterioration of the cement paste. Chloride concentration of the groundwater can also affect the long-term behaviour of the cement paste due to the precipitation of Friedel's salts (i.e. aluminium and calcium chlorides). The formation of Friedel's salts has recently been observed in experiments of chloride penetration (0.5 M NaCl) in concrete performed by /Sugiyama et al. 2008/. Another illustrative example of the effect of the chemistry of the external water on the cement degradation rate is found in /Yamamoto et al. 2007/. In their experiments, they observed the extent of C-S-H replacement for new, Si-richer C-S-H phases as a function of the composition of contacting water (deionised, fresh and saline) in two distinct cements (low-pH grout and Ordinary Portland cement-OPC). After one year of water-cement interaction, the greatest cement modification was observed in the OPC sample in contact with deionised water. In contrast, the low-pH grout did not show significant changes in its composition.

Sulphuric, nitric and organic acid-producing bacteria may degrade concrete /Diercks et al. 1991, Rogers and Hamilton 1993, Monteny et al. 2000/. The sulphuric and nitric acids are produced by bacteria during their litho-autotrophic oxidation of hydrogen sulphide and ammonia. They are mostly known from aerobic environments, but anaerobic variants have been reported as well. Ammonia and hydrogen sulphide are produced during the anaerobic metabolism of denitrifying and sulphate-reducing bacteria (see Section 5.7). This reduction occurs during their consumption of organic compounds. The production, in a two-step process, of inorganic acids from organic material is conceptually possible if the conditions unexpectedly change to aerobic. However, several restrictions in addition to the absence of oxygen will apply, making this a very unlikely scenario in a deep repository. These are: the alkaline conditions expected in concrete environments that may inhibit these microbes as they generally are neutrophilic, the need for some kind of gradient conditions for this two-step reaction to evolve, and that these microbial processes would be most plausible where high concentrations of organic materials exist, which are not expected in a spent fuel repository.

An important effect of the sulphuric acid production is the formation of Ca-sulphates, mainly gypsum and ettringite. The latter is produced by reaction with calcium aluminate hydrate and causes microfracturing due to its very large molar volume (e.g. /Monteny et al. 2000/. This cracking enhances acid penetration into the concrete. Since Ca sulphates are mainly derived from $Ca(OH)_2$ dissolution, the use of low-pH cement (with silica fume as an additive) has proved efficient to lower sulphate attack.

Organic acids can be produced by both bacteria /Diercks et al. 1991/ and fungi /Perfettini et al. 1991/. Anaerobic corrosion of iron and aluminium will produce hydrogen which is an excellent source of energy and electrons for microbes. Acetogenic bacteria are common in deep groundwater /Pedersen 2001/ and they produce acetate from organic compounds or hydrogen (see Section 5.7). This acetate could be used by other organisms, e.g. fungi. Alkalophilic fungal strains have been found to increase cement porosity and reduce the bending strength through their production of gluconic and oxalic acids /Diercks et al. 1991/. Direct contact between the fungal mycelia and the concrete is not necessary for effective dissolution of concrete to take place. These acids are produced during the fungal degradation of organic components. Both fungi and bacteria may be present as they have been detected in deep groundwater /Ekendahl et al. 2003/. In contrast to the inorganic acid-producing microbes, the organic acid producers may be fermentative, which would reduce the requirement for transport of electron-acceptors from outside the repository. High pH in concrete environments may initially reduce such activity /Wenk and Bachofen 1995/, but the absolute upper pH limit for microbial activity is quite high. Data from the natural analogue Maqarin suggest that alkalophilic microbes survive at least up to pH between 12 and 13 /Pedersen et al. 2004/. However, the Maqarin alkalophiles did not demonstrate activity. Results from surface systems such as alkaline lakes suggest that alkalophiles will be active in the 10–11 pH range. When pH goes above 11–12, they may survive, but have to await lower pH before they can be metabolically active.

5.8.2 Dependencies between process and geosphere variables

Table 5-8 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.8.7.

Table 5-8. Direct dependencies between the process "Degradation of grout" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. Mineral-water reactions are temperature dependent.	Excavation/ operation Temperate	Neglected; little significance compared with other influences in expected temperature range.	No.	–	–
		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.			
Groundwater flow	Yes. Mechanical erosion is possible. Also indirectly through groundwater composition by renewal of the groundwater in contact with cement.	All	Mechanical erosion not specifically addressed. Grouting procedures and specifications will prevent erosion.	Yes. By changing permeability of grouted fractures.	All	See Section 3.1 Groundwater flow.
Groundwater pressure	Yes. But, the effect of pressure on chemical reactions is minor. Homogeneous hydrostatic pressure should not affect the mechanical integrity of concrete.	Excavation/ operation Temperate	Neglected; little significance compared with other influences.	No.	–	–
		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.			
Gas phase flow	Yes. Large gas flows may affect the mechanical stability of the grouting.	All	Not specifically addressed. Grouting procedures and specifications will prevent erosion.	Yes. Degraded cement grout might be more permeable for a gas phase flow.	All	See Section 3.2.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Repository geometry	No.	–	–	No.	–	–
Fracture geometry	Yes. It will affect the amount and distribution of grouting.	Excavation/operation Temperate	Generic fracture parameters used in modelling the influence of grout on groundwater compositions.	Yes. Purpose of grouting is to reduce fracture porosity and permeability. Grout degradation reopens fractures.	Excavation/operation Temperate	See Section 3.1.
		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.		Periglacial Glacial	Process not handled.
Rock stresses	Yes. Rock stress might physically break the grouting.	All	Not specifically addressed. Even crushed grout will effectively reduce groundwater flow.	No.	–	–
Matrix minerals	No.	–	–	No.	–	–
Fracture minerals	No.	–	–	No. But indirectly through changes in water composition, e.g. OH^- ions released from cement might generate C-S-H in the fractures.	–	See row Groundwater composition below and Section 5.6.
Groundwater composition	Yes. Affects chemical degradation, e.g. high concentrations of sulphate and chloride ions are detrimental for cement stability. High concentrations of carbonate reduce the rate of cement degradation.	Excavation/operation Temperate	Site-specific Forsmark groundwater composition used in generic modelling of impact of grout on water chemistry.	Yes. Release of OH^- ions from cement will increase groundwater pH locally.	Excavation/operation Temperate	Generic modelling to evaluate changes in composition of groundwater circulating around a grouted fracture and consequent precipitation-dissolution of minerals.
		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	Yes. Grout is a structural material.	Excavation/operation Temperate	Grout composition used for generic modelling of changes in groundwater circulating around a grouted fracture and consequent precipitation-dissolution of minerals.	Yes.	Excavation/operation Temperate	Influence not evaluated; assumptions made regarding grout properties in different applications.
		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.
Saturation	Yes. Cement degradation is negligible in unsaturated rock.	Excavation/operation Temperate	Saturated conditions assumed.	No.	–	–
		Periglacial Glacial	Process not specifically addressed; extrapolation of results from temperate conditions.			

5.8.3 Boundary conditions

Most of the grouting will be performed close to the inner geosphere boundary, that is, near to the repository tunnels, and grout degradation will take place close to repository cavities. A plume of modified groundwater, i.e. higher pH etc, will propagate along the flow path of grouted fractures. However, there are no particular conditions at the geosphere boundaries influencing the degradation of grout. The only relevant conditions for the cement degradation process are related to the chemical composition of the groundwater, which will be the aggressive solution driving the leaching process.

5.8.4 Model studies/experimental studies

A large amount of research has been reported in the scientific literature involving accelerated laboratory leaching tests, among the most recent papers are those of /Faucon et al. 1998, Carde et al. 1996, Saito and Deguchi 2000, Catinaud et al. 2000, Moranville et al. 2004, Yamamoto et al. 2007, Sugiyama et al. 2008/. Experimental evidence has also been reported on long-term leaching through the analysis of old, man-made, cementitious structures /Álvarez et al. 2000, Lagerblad 2001/.

Model prediction of cement degradation has been a challenge due to the strong incongruent dissolution and replacement of C-S-H gels. After portlandite dissolution, Ca-rich C-S-H starts to transform into a new Si-rich C-S-H, coupled with a decrease in pH. The initial modelling approaches used a (usually) small number of crystalline C-S-H phases (14Å tobermorite, Ca/Si = 0.83; Jennite, Ca/Si = 1.5) in thermodynamic equilibrium with the cement porewater. A flaw in these approaches was the inability to precisely model the incongruent dissolution of the C-S-H. Another approach has been the consideration of the C-S-H phases as solid solutions. This was adopted since it is an elegant way to model incongruent dissolution. However, C-S-H are not solid solutions; actually, they are not crystalline solids, which is an imperative requirement for a solid solution. In addition, crystalline equivalents of C-S-H are not proved to be solid solutions. Many recent studies have used solid solutions to model cement degradation (e.g. /Berner 1988, 1992, Kersten 1996, Börjesson et al. 1997, Rahman et al. 1999, Kulik and Kersten 2001, Sugiyama and Fujita 2006, Carey and Lichtner 2007, Walker et al. 2007/). Most of them assumed a strong non-ideality of the solid solution series (meaning that the solubility constant of a C-S-H member depends not only on its molar fraction but also on the composition of the solid itself).

The complex nature of the C-S-H system is reflected in the fact that it has proved impossible to reproduce the degradation of the C-S-H in the whole Ca/Si range of compositions (commonly 0.5–2.5) by considering only two end-members and fixed interaction parameters. This is true at least when dealing with the data trend shown by the /Harris et al. 2002/ dataset type. /Berner 1988, 1992/ used three different end-members to calculate the apparent solubility product of the C-S-H phases. The end-members were SiO_2, CaH_2SiO_4 and $Ca(OH)_2$. In following works /Börjesson et al. 1997, Rahman et al. 1999, Walker et al. 2007/ used two end members ($Ca(OH)_2$ and CaH_2SiO_4) and two interaction parameters but the model can only reproduce C-S-H phases with Ca/Si>1, excluding the alteration of low-pH cements. Later, /Kulik and Kersten 2001/ selected two binary, ideal solid solutions (C-S-H-I and C-S-H-II) based on structural calculations. C-S-H-I considers SiO_2 and tobermorite-I, and C-S-H-II has as end-members tobermorite-II (with the same formula as tobermorite-I but different solubility constant) and jennite. The solubility products of the end-members were optimised to fit the experimental data by modifying the number of Si moles in the structural formula. /Sugiyama and Fujita 2006/ calculated the corresponding conditional solubility constants for four groups of C-S-H compositions considering only two end-members, $Ca(OH)_2$ and SiO_2, covering the whole Ca/Si range. They used variable interaction parameters for the C-S-H with compositions above and below Ca/Si = 0.833. This model was subsequently used by /Benbow et al. 2007/ in a reactive transport model of a cement block. Also, /Grandia et al. 2010/ used the /Sugiyama and Fujita 2006/ approach to reproduce the experimental data of leaching experiments performed by /Yamamoto et al. 2007/. Finally, /Carey and Lichtner 2007/ succeeded in reproducing the experimental data of /Chen et al. 2004/. They found that the C-S-H composition and the solution in equilibrium could be explained using a solid solution model with $Ca(OH)_2$ and SiO_2 as end-members and only three (invariable) interaction parameters. This model adequately predicts the degradation of high-pH C-S-H, but is less successful at low Ca/Si ratios.

Recent models of cement degradation have addressed the task of considering the effects of evolution of physical properties (i.e. porosity, diffusivity) on the behaviour of the leaching process. Some of them on the basis of fitting curves derived from experimental data /Yokozeki et al. 2004/ and some others on either "pure" random models /Bentz and Garboczi 1992/ or "hybrid" models, where randomness is constrained by appropriate user-defined probability distributions /Marchand et al. 2001/. A pure mechanistic approach for cement degradation modelling requires the coupling of multi-component solute diffusion and chemical reactions taking place in the system. Dimensionless analyses of diffusion and reaction rates demonstrate the adequacy of a local equilibrium assumption for coupled reactive transport modelling of cement leaching /Barbarulo et al. 2000/. By this approach, a mixed non-linear set of equations can be solved numerically. The domain of the problem could be represented either as a homogeneous medium, obtained by averaging the variables of interest over a representative elementary volume, or a pore structure modelled on the basis of microstructural information, such as that provided by mercury intrusion porosimetry, or on the reconstruction of the microstructure by means of random models /Bentz 1999/. The latter was recently addressed in /Moranville et al. 2004, Galíndez et al. 2006, Galíndez and Molinero 2010/.

A relevant decision to be taken in the reactive transport-based models of cement degradation arises from the selection of the geochemical processes to be included. The inclusion of K^+, Na^+, Mg^{2+}, Ca^{2+}, SO_4^{2-}, OH^-, $Al(OH)_4^-$ and Cl^-, is claimed in /Maltais et al. 2004/ to be sufficient to describe most degradation processes, although other sets of chemical components have also been proposed, e.g. in /Höglund 2001/.

5.8.5 Natural analogues/observations in nature

C-S-H gels in nature are rare. The best examples are found at Maqarin (Jordan), where natural combustion of carbonate rocks resulted in the formation of calcium-silicate minerals. The hydration of these minerals led to C-S-H gels that caused hyperalkaline springs when interacted with meteoric waters /Linklater 1998, Smellie 1998/. Other examples can be found in contact metamorphic zones associated with skarns (metamorphic calc–silicate rocks) /Milodowski et al. 1989/ and in amygdales in mafic igneous rocks /Walker and Bloem 1960/.

Little information on grout durability is revealed from natural studies. However, the co-existence of gel-like C-S-H and more ordered, crystalline phases at Maqarin suggests a very low rate of transformation ("ageing"), covering geological time scales.

5.8.6 Time perspective

Since cement leaching is a coupled diffusion-reaction phenomenon, the time needed for complete degradation of cement grout will be highly dependent on the relative surface area of the grout where diffusion with groundwater can take place. This parameter will be related to the thickness of the grout, which will be much larger in grouted boreholes than in the grouted fractures. /Höglund 2001/ performed reactive transport calculations to simulate grout degradation. The calculations assumed molecular diffusion as the only transport mechanism within the grout. The author found that the time perspective for grout degradation can be estimated to 10,000 years. Also, the initial porosity of the grout is a relevant parameter since it limits the diffusion of ions in and out of the grout porewater.

5.8.7 Handling in the safety assessment SR-Site

This process does not need any detailed modelling in SR-Site in view of the fact that the quantities are relatively small and that "low-pH" cement grouting will be used.

Excavation/operation

The process is not specifically addressed for the excavation/operation period, since the expected effects will occur during temperate conditions. Some alteration will take place initially during the operation phase, but most of the leaching porewater will be mixed with the groundwater infiltrating the tunnel and, thus, be pumped away.

Temperate climate domain

After closure the grout will reacting with the groundwater and thereby increase the pH locally and create an alkaline plume that will progress downstream. The effect of "low pH" shotcrete and grouting on the chemistry of fractures surrounding the repository tunnels is evaluated through generic numerical calculations. In the modelling, groundwater is allowed to flow in a fracture around grouted areas, causing dissolution of calcium silicate hydrates, and the consequent chemical changes downflow of the grouted area are evaluated /Grandia et al. 2010/.

Periglacial- and glacial climate domains

The process is not specifically addressed for periglacial- and glacial conditions. However, the effects are estimated by extrapolation of the results from the generic modelling for temperate conditions.

Earthquakes

Fracturing, e.g. as a consequence of seismic activity, could accelerate grout degradation. This has not been studied in SR-Site and is thus not handled. However, the possibility that this would have happen, is very low.

5.8.8 Uncertainties

Uncertainties in mechanistic understanding

A main uncertainty is that the thermodynamic and physical properties of gel-like C-S-H are poorly known. This has led to an oversimplification of the predictive models of cement degradation. As an example, the molar volumes used in modelling are extrapolated from the crystalline analogues. This parameter is of fundamental importance since it controls the long-term pore connectivity in the grout during the C-S-H replacement process. In turn, connected porosity plays an important role in the diffusivity which is the driver of geochemical reactions in the grout.

There are also uncertainties regarding the quantities of materials that remain and where in the repository they are. Approximate total quantities can be estimated today. Where they are concentrated and how in relation to each other may be of importance to future safety assessments. These will likely be periodic safety assessments that will occur during repository construction and operations.

Model simplification uncertainties in SR-Site

The calculations to evaluate the effect of "low pH" grouting on the chemistry of fractures surrounding the repository tunnels are made using a simplified geometry (single fracture plane transecting a tunnel) and neglecting matrix diffusion. Furthermore, the solid phases considered are a simplification of the C-S-H phases that precipitate in reality.

Mechanical stability has little effect on grout function.

Input data and data uncertainties in SR-Site

The main uncertainties concern the possible geometrical distribution of grout in fractures, the composition of the grout paste and the thermodynamic stability of calcium-silicate-hydrates.

5.8.9 Adequacy of references supporting the handling in SR-Site

Most of the cited references correspond to peer-reviewed papers published in the top scientific journals of the field. The main scientific references are cited in the SKB report by /Grandia et al. 2010/ that is a report that has undergone a documented factual review.

5.9 Colloidal processes

5.9.1 Overview/general description

Colloids, particles with diameters between 1 and 1,000 nm, have large specific areas, giving them a high affinity for different contaminants in natural systems. Multivalent metal ion sorption on natural colloids is promoted by the existence of negatively charged surfaces on colloidal clays and organic degradation products in neutral to alkaline pH, as well as specific chemical reactions with surface sites. In the case of canister failure, actinides will be strongly adsorbed to the montmorillonite buffer. If the bentonite barrier were to be in contact with groundwater having low ionic strength, montmorillonite colloids would be released and radionuclides transported out of the repository /Wold 2010/. Depending upon particle density, smaller colloids remain in stable suspension for very long times because Brownian motion prevails over gravitational forces. Stability in combination with high sorption capacities, gives colloids an important role in the transport of contaminants, particularly those with low solubility. A well-known example is the colloid-facilitated plutonium migration at the Nevada Test Site /Kersting et al. 1999/. In a deep bedrock repository, there are different classes of colloids that could be present. In groundwater, natural colloids form by the erosion of rock-forming minerals and alteration products, the precipitation of mineral oxides and the degradation of organic material. A special group of colloids includes viruses (2 to 80 nm) and bacteria (200 nm to several microns). Bentonite is in itself colloidal, and can under certain conditions be a colloidal source. Also the bentonite contains a small amount of organic material, which can be leached out in colloidal form /Vilks et al. 1998/. A special class of colloids are the eigencolloids formed by precipitation of metal ions, which would be most likely to occur in close proximity to the spent fuel in a canister. Metal ions with high charge, such as Al^{3+}, Fe^{3+}, Pu^{4+}, Th^{4+} etc, are strongly hydrolysed at pH values prevailing in groundwaters. The hydrolysis products contain several metal ions (i.e. they are polynuclear) and by aggregation they can form colloidal particles. In the case of Pu, the formation of colloids is practically irreversible at the timescales studied in experiments.

For colloids to contribute to contaminant transport, they have to be mobile, remaining in stable suspension for long time periods. The stability of colloids is determined mainly by the groundwater composition, where ionic strength and pH are the most dominating factors /García-García et al. 2006, 2007/. Also temperature, exposure to irradiation and the presence of other colloids will influence colloidal stability. Due to different properties, the dependences are colloid specific. The critical coagulation concentration (CCC) is a measure of colloid stability that is often used to estimate the potential of a given groundwater to carry significant amounts of colloids. A total cation concentration value that is over or equal to the CCC represents unfavourable conditions for colloid stability, i.e. the aggregation is diffusion controlled and appears to be an instantaneous process. CCC-values in the magnitude of 0.1 M Na^+ for Na-montmorillonite and 0.001 M Ca^{2+} for Ca-montmorillonite are reported /García-Garcia et al. 2007/. Stability experiments with montmorillonite including both Ca and Na as counter ions indicate that the CCC-value is a complex concept, since the critical Na-concentration depends on the Ca-concentration and *vice versa*. Therefore, the authors suggest that a single CCC-value should not be used, but a combined CCC-value for the Ca- and Na-concentrations obtained from the diagram of the possible sol formation zone, shown in Figure 7-3 in /Birgersson et al. 2009, page 116/. Montmorillonite colloids are particularly unstable in the presence of concentrations of divalent cations such as Ca^{2+} and Mg^{2+} /Degueldre et al. 1996/. The CCC values in the literature match the general finding at the Grimsel test site where the natural colloid concentrations are less than 10^{-4} g/L (for colloids > 100 nm) at groundwater concentrations of $Ca^{2+} \geq 10^{-4}$ M or $Na^+ \geq 10^{-2}$ M /Degueldre et al. 1996/. In an inventory of groundwaters at the Äspö HRL, where the ionic strength ranges from 0.1–0.6 M, the measured colloid concentrations never exceeded 300 µg/L in shallow and 50 µg/L in deeper groundwaters at repository depth /Laaksoharju and Wold 2005/.

In the deep groundwaters at the Laxemar and Forsmark sites, the salinities far exceed the concentrations required for natural or bentonite colloids to be stable /Auqué et al. 2006/. The measured low concentrations of natural colloids confirm the existing unfavourable conditions for colloidal stability. Intrusion of atmospheric oxygen in a reducing groundwater may give rise to extensive colloid formation. Immediately after closure of the repository, Fe (II) dissolved in the groundwater will react with dissolved oxygen and entrapped air, mostly in the buffer and backfill, but also with small amounts in the excavation damaged zone (EDZ) and in the rock matrix and around the tunnel walls. This chemical reaction will produce colloidal Fe(III) oxyhydroxides. As a result, the water may contain high concentrations of colloidal material during a transitional period, in the order of several to several tens of mg/L /Wikberg et al. 1987/. A small contribution is expected from grout and other cement materials /Wieland et al. 2004/. The colloid concentrations will most probably decrease to low values in a short time, due to the high salinities in the surrounding groundwater. The relatively high Ca^{2+} content in the contact water contributes to the stabilisation of the cement. The recovery of colloid concentrations in Äspö waters after injection of colloidal Silicasol for fracture sealing is currently followed in the Colloid Transport Project. As long as the groundwater has a high ionic strength with a high content of divalent cations such as Ca^{2+} or Mg^{2+} it is unlikely that colloidal transport will be significant. This is supported by results of colloid migration tests in a fracture with an aperture of mm-size where injected bentonite colloids readily aggregated and sedimented out from solution in synthetic Äspö groundwater /Vilks et al. 2008/.

As a result of future climate changes, the hydrological conditions may alter, which, in turn, may significantly affect groundwater chemistry. In Sweden, as in the other Nordic countries, glacial cycles can be expected in the future. During melting and retreat of the ice sheet, it cannot be excluded that melt water will intrude to repository depth in water-conducting fractures, thereby displacing the existing saline groundwater. In this scenario, colloid transport is assumed to take place. The bentonite buffer in contact with dilute water in water-bearing fractures can plausibly release bentonite colloids. Since montmorillonite colloids are known to be stable in dilute waters, bentonite-based barriers may start to erode, followed by bentonite colloid transport away from the barrier /Missana et al. 2003/. Bentonite erosion and the potential release of bentonite colloids are further discussed in the Buffer, backfill and closure process report /SKB 2010e/.

If the uptake of radionuclides on colloidal particles is reversible, the impact of colloids on radionuclide transport will likely be negligible. If, on the other hand, the radionuclides adhere irreversibly, the situation will be different. In this case, radionuclides with low solubility will be transported mainly with the particles and, at worst, not be delayed by either sorption on fracture walls or by matrix diffusion in the rock.

Colloids can be transported slightly faster than conservative tracers in water-bearing fractures. This has been observed e.g. in the Colloid and Radionuclide Retardation experiment at the Grimsel test site. Early breakthrough for Am sorbed to bentonite colloids compared to the non-sorbing tracer ^{131}I is explained by hydrodynamic chromatography effects, i.e. the colloids are taking the fast track in the middle of the fracture, whereas the tracers are transported in the whole flow profile, even close to the walls /Kurosawa et al. 2006/. The sorptivity of actinides, fission products and activation products on bentonite and minerals have been well studied. However, few data on desorption are available, and also very few on sorption/desorption to the colloidal fraction, particularly on the longer timescales that are relevant for transport processes in the geosphere. This information is essential for knowing whether or not sorption should be treated as a reversible process when modelling the effect of colloids on radionuclide transport /Alonso et al. 2006/.

Bentonite erosion may not necessarily result in significant colloid transport away from the buffer. The bentonite contains accessory minerals that are larger and denser than the montmorillonite colloids. A possible scenario is that they will sediment rather quickly in the water bearing fracture and then act as a filter for the eroded colloids. That may make the system self sealing. Further colloid filtration and retardation processes in the system depend on a number of factors such as flow velocity, aperture distribution, surface roughness, mineral composition, and colloid characteristics, namely size distribution, conformation, surface charge and particle density. The flow velocity is plausibly the most determining factor. At high flow rates, such as those used in field-scale tracer tests, filtration of colloids may not be important. At low flow rates, similar to natural flow rates in water-bearing fractures, filtration may be very significant. The filtration of particles in natural systems can be classified as straining filtration or as physical-chemical filtration /McDowell-Boyer et al. 1986, Yao et al. 1971, Moridis et al. 2003/. Physical-chemical filtration occurs when colloids are significantly smaller than the pore diameters or the fracture apertures. In this case, particle retardation can only occur when particles collide with and stick to rock surfaces. The probability of particle collisions with the geological media is determined by the particle size and density (and flow velocity). Sedimentation (of large particles) and diffusion (of small particles) as well as hydrodynamic effects will determine the contact between the colloids and the fracture wall /Moridis et al. 2003/.

The ability of particles to stick to fracture surfaces is influenced by the ability of colloids to sorb onto mineral surfaces. Even though the overall mineral surface is negatively charged at neutral pH, charge distribution is heterogeneous and some mineral surfaces may have a local positive charge where sorption can take place. Clays, for example, have multiple surface charges, some of which are pH dependent. Colloid sorption behaviour is still not well understood, and sorption of colloids may occur even under unfavourable conditions /Alonso et al. 2006/. Another possibility is that films of organic degradation products, or bacteria, change the fracture surface charge and surface characteristics. Migration tests in a granite block with a fracture in the mm-range reveal differences in transport according to conformation and density. Latex and bentonite colloids, in the same size and surface charge ranges, are transported differently at low flow velocity. Latex colloids more readily travel in the fracture, and the recoveries are significantly higher than for the bentonite colloids /Vilks et al. 2008/. The effects of fracture and colloid characteristics on colloid transport in water-bearing fractures are addressed in the Colloid Transport Project. The main goal is to identify and quantify the impact of the different parameters to be able to perform predictive modelling for colloid transport on different scales.

5.9.2 Dependencies between process and geosphere variables

Table 5-9 shows how colloidal processes are influenced by and influence all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.9.7.

Table 5-9. Direct dependencies between "Colloidal processes" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. Preliminary laboratory studies show that bentonite colloid stability is temperature dependent.	All	Process neglected; insignificant impact on geochemical conditions.	No.	–	–
Groundwater flow	Yes. Gravitational settling will be affected by flow velocities. Colloid filtration will be highly dependent on the flow. Furthermore, although the flow will not affect colloids in itself, colloids might form when groundwaters mix and by erosion.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. See Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.	No.	–	–
Groundwater pressure	No.	–	–	No.	–	–
Gas phase flow	No. Colloids do not form in a gas phase. Even though it cannot be excluded that colloids are transported as aerosols, the effect may be neglected. Indirectly, flow of a reactive gas phase, e.g. air, will result in the oxidation of any dissolved Fe(II) and in the subsequent precipitation of Fe(III)-oxyhydroxide colloids.	–	–	No. Colloids in themselves do not affect the gas phase. The reactions producing colloids might affect the composition of the gas phase, e.g. the oxidation of dissolved Fe(II) by air will deplete oxygen from the gas phase. The gas flow should remain mainly unchanged.	–	–
Repository geometry	No.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture geometry	Yes. The geometry of the fractures will affect the colloid transport and their retention mechanisms. In finer fractures, the colloids will interact to a greater extent with the fracture surfaces by physical filtration and electrostatic attachment than in larger fractures.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. See Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.	No.		
Rock stresses	No.	–	–	No.	–	–
Matrix minerals	No.	–	–	No.	–	–
Fracture minerals	Yes. Colloids might form by resuspension of e.g. clays in very dilute waters. Attachment of colloids to fracture minerals is important.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. See Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.	Yes. Suspended colloids might sediment onto fracture walls, e.g. when groundwaters mix.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. Influence neglected; little significance. See also Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.
Groundwater composition	Yes. Concentration of dissolved salt affects the stability of colloids. pH and the presence of organic materials can affect the stability of colloids. Colloids might form by precipitation from oversaturated solutions.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. See Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.	Yes. Precipitation of colloids from oversaturated solutions will change the composition of the groundwater.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. See Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.
Gas composition	No. Colloids do not form in a gas phase. However, a reactive gas phase, e.g. oxygen in air, in contact with a groundwater will result in the oxidation of any dissolved Fe(II) and in the subsequent precipitation of Fe(III)-oxyhydroxide colloids.	–	–	No. Colloids in themselves do not affect the composition of a gas phase. However, the reactions producing them might, e.g. the oxidation of dissolved Fe(II) by air will deplete oxygen from the gas phase.	–	–
Structural and stray materials	Yes. Concrete releases only a small amount of colloids /Wieland et al. 2004/, but organic matter may degrade and form organic colloids.	Excavation/ operation Temperate Periglacial Glacial	Process neglected; insignificant impact on geochemical conditions. Influence neglected; little significance. See also Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Saturation	Yes. Colloids do not form in a gas phase. A reactive gas phase, e.g. oxygen in air, in contact with a groundwater will result in the oxidation of any dissolved Fe(II) and in the subsequent precipitation of Fe(III)-oxyhydroxide colloids.	Excavation/ operation	Process neglected; insignificant impact on geochemical conditions.	No.	–	–
		Temperate Periglacial Glacial	Influence neglected; little significance. See also Section 6.1 Radionuclide transport and Montmorillonite colloid release in Buffer, backfill and closure process report /SKB 2010e/.			

5.9.3 Boundary conditions

The exchange of solutes with the biosphere, with remote parts of the geosphere and with buffer/backfill in the repository comprises the boundary conditions for the formation and stability of colloids. Climate change will lead to changes in the composition of the water entering the geosphere, which, in turn, may lead to long-term changes in groundwater composition, thus affecting the stability of colloids. The boundary conditions for colloid transport are the same as those for transport of other solutes (see Section 6.1).

5.9.4 Model studies/experimental studies

Colloids have been modelled and investigated experimentally in many different contexts, including a EU project with participants from a number of research institutes /Kim et al. 1996/. Under reducing conditions in the bedrock, the concentrations are usually so low that they are difficult to measure. A value of 50 µg/L was estimated on the basis of an evaluation of measured concentrations and an estimate of the uncertainties inherent in these values. The evaluation is based on an experimental study conducted in cooperation between SKB and TVO at Olkiluoto /Laaksoharju et al. 1993/. This value compares well with the levels measured at Äspö, Laxemar and Forsmark. The colloid content in different Äspö groundwaters was measured to be less than 300 µg/L, and less than 50 µg/L at repository depth /Laaksoharju and Wold 2005/. The total range of measured colloid concentrations in Forsmark is 5–170 µg/L and the average is 58 µg/L /Laaksoharju et al. 2008b/ and for Laxemar the range is 5–90 µg/L and the average is 24 µg/L /Hallbeck and Pedersen 2008c/. These values compare with those from studies of colloids in crystalline rock groundwaters in Switzerland (30 and 10 µg/L /Degueldre 1994/).

In the colloid dipole experiment at the Grimsel test site, radionuclides with and without bentonite colloids were injected in one borehole and collected in another borehole, which was communicating with the first hole through a fracture. The experiment indicates that bentonite colloids enhance radionuclide transport /Möri et al. 2003b/. The groundwaters at Grimsel are very dilute (~ 10^{-3} M ionic strength) and the pH is around 9. Under these conditions, natural colloids and bentonite colloids are very stable. The conditions in the groundwaters at Äspö (representative of deep Swedish granitic groundwater) are very different, with high concentrations of both Na^+ and Ca^{2+} and with pH values of between 7 and 8. In these groundwaters, colloid stability is very low. At repository depth, Na and Ca concentrations range between 500 and 3,000 and between 500 and 2,000 mg/L, respectively, for Laxemar /Gimeno et al. 2008/ and for Forsmark the corresponding concentration ranges are 1,200–2,200 mg/L for Na and 1,000–3,000 mg/L for Ca /SKB 2008a/.Although it could be argued that the low ionic strength conditions at the Grimsel site are analogous to the expected meltwaters during future glaciation periods, it is known that the sedimentation of colloids is strongly dependent on groundwater flow. In that respect, the *in situ* colloid enhanced radionuclide transport experiment at Grimsel was unrealistic. It must also be noted that the natural concentration of colloids in Grimsel waters is quite low.

Colloid stability and transport of especially bentonite colloids in dilute water mimicking glacial water, on different scales, has been performed in the SKB Colloid Dipole Project, and is further carried on in the SKB Colloid Transport Project /García-García et al. 2006, 2007, Vilks et al. 2008/. In the ongoing Grimsel Colloid Formation and Migration (CFM) project conducted at the Grimsel Test Site, bentonite erosion is studied on metre to field scales. The purpose is to investigate the influence of colloids on radionuclide migration in a fractured host rock under advective flow conditions at repository relevant conditions.

5.9.5 Natural analogues/observations in nature

In addition to the references given in the section "Overview/general description" above, colloids have been addressed in most of the major international natural analogue studies, for example, Poços de Caldas, Brazil /Miekeley et al. 1992/, Cigar Lake, Canada /Vilks et al. 1991/, Oklo, Gabon /Gauthier-Lafaye et al. 2000/, Palmottu, Finland /Blomqvist et al. 2000/ and Maqarin, Jordan /Smellie 1998/. These studies show that it is necessary to study the presence of colloids at potential nuclear waste repository sites.

5.9.6 Time perspective

Extensive colloid formation can be expected in conjunction with closure of the repository, when mixing of oxidising and reducing waters occurs. The time this takes is determined by the groundwater flow and it may range from a few years to several hundreds of years, depending on the hydraulic properties of the site.

The stability of colloids, originating for example from the bentonite in the buffer, would increase if extremely dilute waters passed through the repository. During a glaciation, melt waters under the ice sheet might be forced down to repository depth. If these waters contain large amounts of dissolved oxygen they will induce the oxidation of Fe(II) in near-surface waters, resulting in colloidal Fe(III) oxyhydroxides. Although these melt waters are very dilute initially, which would stabilise colloids, they are expected to acquire solutes during their travelling time in the fractures by reactions with minerals present in the fracture surfaces, causing colloids to sediment.

The time perspective for colloid-facilitated radionuclide transport can be considered to be the same as that for advective radionuclide transport (see Section 6.1).

5.9.7 Handling in the safety assessment SR-Site

Colloids have negligible impact on the geochemical conditions of the geosphere. However, colloids may act as carriers for radionuclides released from the spent fuel. In a study by /Allard et al. 1991/, the colloids were assessed to be of no importance for radionuclide transport even for colloid concentrations of 0.5 mg/L. Colloid-mediated radionuclide transport is further discussed in Section 6.1.

Excavation/operation period

Extensive colloid formation is expected to occur temporarily in connection with the closure of the repository. Shortly after closure and from then on, the majority of colloids will sediment and a maximum pessimistic value for the concentration of colloids is 0.5 mg/L /Laaksoharju et al. 1995a/.

Temperate-, periglacial- and glacial climate domains

The concentration of colloids should be low to prevent colloid-mediated transport of radionuclides. The current salinities of the groundwaters at both Forsmark and Laxemar are higher than that required to keep the concentration of colloids suspended in groundwaters to a low level. However, future changes in groundwater composition may imply less saline waters and, especially, melt waters from an inland ice sheet may have low concentrations of dissolved salts. Such waters could stabilise colloids and erode the bentonite buffer and the deposition tunnel backfill. Analyses of release of colloids from buffer and deposition tunnel backfill will be undertaken if the total charge concentration of cations in the groundwater is 4 mM or less. This is further described in the process report for Buffer, backfill and closure /SKB 2010e/. The handling of transport in the geosphere of radionuclides attached to colloids is described in Section 6.1.

Earthquakes

The impact of earthquakes on colloid-mediated transport is not specifically addressed since geosphere retardation is cautiously disregarded in the analyses of impacts of earthquakes. This is further described in Section 6.1.7.

5.9.8 Uncertainties

Uncertainties in mechanistic understanding

Formation of colloids is dependent on several factors that currently are not fully understood. Colloids are by definition thermodynamically metastable and consequently their occurrence and stability cannot be approached from an equilibrium point of view.

Model simplification uncertainties in SR-Site

See Section 6.1.8.

Input data and data uncertainties in SR-Site

See Section 6.1.8.

5.9.9 Adequacy of references supporting the handling in SR-Site

The supporting references in this section are both peer-reviewed scientific papers and SKB reports. The SKB reports have undergone documented factual and quality reviews, although the reviews of the older ones were not documented according to SR-Site standards.

5.10 Formation/dissolution/reaction of gaseous species

Gaseous species are taken to be substances that exist as gases under the range of temperatures and pressures that include those of the repository and ambient conditions. This section deals with the microbiological and chemical (abiotic) formation and reaction processes in which the gases dissolved in groundwater may be involved in the geosphere. About 15 different gases can be expected at various concentrations above trace amounts (dissolved in the groundwaters) in the geosphere surrounding a repository /Pedersen 2001, 2002, Hallbeck and Pedersen 2008a, b, c, Pedersen et al. 2008/. The influence of geosphere variables on gaseous species processes and the converse varies significantly from none to a large influence.

The process of formation and the place of origin differ for different geosphere gases. They can be biological processes in the atmosphere, radioactive decay at different places or thermogenic, chemical processes in deep crustal and mantle layers of the Earth. Several gases have a primordial origin, meaning that they were formed before the Earth was formed; they were aggregated during the condensation of the Earth, and have been degassing to the atmosphere, through the geosphere since then. In this section, the place of origin for each gas is identified together with the main processes of formation. Important reactions of geosphere gases are also discussed. The place of origin is represented by four different environments (Table 5-10).

The atmosphere here includes all places above the ground surface where oxygen is present, including photosynthetic organisms and aquatic environments. The geosphere is defined by the boundary conditions as described in Section 5.10.3. The repository with construction materials, buffer and canisters is defined as engineered areas. Deep crustal and mantle areas, below the defined geosphere area, are denoted deep layers. The formation of gases has been categorised according to main processes. Radioactive decay is by far the most diverse process, which explains formation of specific gases in part or completely. Here, only decay processes judged to be important for repository performance are included. It is out of the scope of this process section to deal with detailed decay series that generate trace gases, such as, for example, radon. Anaerobic corrosion of metals in the engineered area and several processes that include mineral interactions can also generate gases. Finally, a number of gases can, in addition to radioactive, thermogenic and chemical processes, be produced by biological processes. Oxygen is almost exclusively produced by biological photosynthetic processes.

5.10.1 Overview/general description

The characteristics of the different gases likely to be present in solution in groundwater at a repository site (Table 5-10) are briefly described here. Focus is on their place of origin, processes of formation and what reactions they may be part off. The reactions of dissolved gases in the geosphere should be considered alongside the reactions of other dissolved compounds; there is no fundamental difference between the two. Solubility and dissolution issues are discussed under a common heading for all gases. There are significant differences between chemical and biological formation and reaction processes. Several important reactions, such as the formation of methane and the reduction of nitrate to nitrogen gas, are very slow or do not occur at all under the temperature and pressure conditions typical of a repository. Such reactions are, however, performed by microorganisms via biochemical pathways that can bypass activation energy barriers and other thermodynamically related, reaction inhibiting, properties of these reactions /Madigan and Martinko 2006/. Biological and chemical processes in the geosphere are, therefore, separated below. The conditions for these reactions are set by the expected temperature and pressure range conditions in the geosphere.

Table 5-10. Gases that can be found in the geosphere, their places of origin and processes of formation, and components included in major geosphere reactants and end products. Solubility of each gas is given for atmospheric pressure and 20°C /Aylward and Findlay 2002/.

Gas	Places of origin	Processes of formation	Solubility (mL L^{-1})	Major geosphere reactants and end products	
				Chemical	Biological
H_2	Atmosphere	–	17.9	–	$H_2 + O_2 \rightarrow H_2O$
	Geosphere	Radiolysis, fermentation.			$H_2 + CO_2 \rightarrow CH_4$
	Repository	Anaerobic corrosion of metals.			$H_2 + CO_2 \rightarrow CH_3COOH$
	Deep layers	Radiolysis, cataclasis, hydrolysis, serpentinisation. Primordial origin.			$H_2 + SO_4 \rightarrow H_2S$ $H_2 + Fe^{3+} \rightarrow Fe^{2+}$
He	Atmosphere	–	16.8	–	–
	Geosphere	Radioactive decay			
	Repository	Radioactive decay.			
	Deep layers	Radioactive decay. Primordial origin.			
Ne	Atmosphere	Radioactive decay.	14.7	–	–
	Geosphere	Radioactive decay.			
	Repository	–			
	Deep layers	Radioactive decay. Primordial origin.			
Ar	Atmosphere	Radioactive decay.	73.4	–	–
	Geosphere	Radioactive decay.			
	Repository	–			
	Deep layers	Radioactive decay. Primordial origin.			
O_2	Atmosphere	Photosynthesis.	30.4	$O_2 + Fe/Fe^{2+} \rightarrow Fe^{3+}$	$O_2 + Fe^{2+} \rightarrow Fe^{3+}$
	Geosphere	–		$O_2 + S^{2-} \rightarrow SO_4^{-2}$	$O_2 + S^{2-} \rightarrow SO_4^{-2}$
	Repository	–			$O_2 + H_2 \rightarrow H_2O$
	Deep layers	–			$O_2 + CO \rightarrow CO_2$
					$O_2 + CH_4 \rightarrow CO_2$
					$O_2 + (CH_2O)_n \rightarrow CO_2 + H_2O$
N_2	Atmosphere	–	15.2	–	$N_2 + ATP^1 \rightarrow -NH_2$
	Geosphere	Biological denitrification.			
	Repository	–			
	Deep layers	Primordial origin.			
CO	Atmosphere	Combustion.	22.7	–	$CO + O_2 \rightarrow CO_2$
	Geosphere	Degradation of organic			CO + enzymes $\rightarrow CH_3COOH$
	Repository	compounds.			CO + enzymes $\rightarrow CH_4$
	Deep layers	Degradation of organic compounds. Mantle and crustal processes.			

Gas	Places of origin	Processes of formation	Solubility (mL L^{-1})	Major geosphere reactants and end products	
				Chemical	Biological
CO_2	Atmosphere	Respiration, combustion	860	Dissolution	$CO_2 + H_2 \rightarrow CH_4$
	Geosphere	Respiration, combustion		Weathering	$CO_2 + H_2 \rightarrow CH_3COOH$
	Repository	Respiration, combustion			
	Deep layers	Mantle and crustal processes, dissolution of carbonates.			
H_2S	Atmosphere	–	2,540	H_2S + Me[2] $\rightarrow$ MeS	$H_2S + O_2 \rightarrow SO_4^{2-}$
	Geosphere	Biological sulphate reduction			
	Repository	Biological sulphate reduction			
	Deep layers	Biological sulphate reduction Thermogenic processes			
CH_4	Atmosphere	–	32.2	–	$CH_4 + O_2 \rightarrow CO_2$
	Geosphere	Biological methanogenesis			$CH_4 + SO_4^{2-} \rightarrow H_2S$
	Repository	Biological methanogenesis			
	Deep layers	Biological methanogenesis Serpentinisation Thermogenic processes			
C_2H_6	Atmosphere	–	46.3	–	–
C_2H_4	Geosphere	–	119		
C_2H_2	Repository	–	101		
$C_3H_{4–8}$	Deep layers	Thermogenic processes			

[1] ATP = adenosine-tri-phosphate; [2] Me = Metal

Hydrogen

Hydrogen is the most abundant element in the universe and consists of three isotopes with mass number 1, 2 and 3. Hydrogen gas (H_2) is explosive in oxygenic environments and can act as a strong reducing agent as is revealed by the negative redox potential of hydrogen.

H_2 can be formed in microbiological or biological fermentation processes and by a range of different processes not involving life. Fermentation occurs in anaerobic systems such as water-logged soils and anoxic groundwater, i.e. in the geosphere. Fermentative processes cannot produce high concentrations of hydrogen /Madigan and Martinko 2006/; hydrogen produced during fermentation is commonly combined with carbon dioxide to methane by methanogens. The radiolysis of water has been proposed by /Lin et al. 2005/ as a possible H_2 generation process occurring in the Precambrian granitic system including the Fennoscandian Shield (yield rate calculated to $9.4·10^{-9}$ nM s^{-1}). Radiolysis of water to oxygen and H_2 can consequently produce small amounts of H_2 in the geosphere, but the main natural source of hydrogen to the geosphere is likely transport from deep layers by diffusion and advection. Anaerobic corrosion of metals, mainly iron and steel, in the engineered areas will also produce H_2, as will corrosion of the cast iron insert in canisters that fail and take in water.

There are at least six possible processes by which crustal H_2 is generated: (1) reaction between dissolved gases in the C-H-O-S system in magmas, especially in those with basaltic affinities; (2) decomposition of methane to carbon (graphite) and hydrogen at temperatures above 600°C; (3) reaction between CO_2, H_2O, and CH_4 at elevated temperatures in vapours; (4) radiolysis of water by radioactive isotopes of uranium and thorium and their decay products and by radioactive isotopes of potassium; (5) cataclasis of silicates under stress in the presence of water; and (6) hydrolysis by ferrous minerals in mafic and ultramafic rocks /Apps and van de Kamp 1993/.

Chemical reactions: H_2 is not expected to react chemically at significant rates under repository conditions.

Biological reactions: H_2 is an important gas in several anaerobic microbial metabolisms in deep groundwater, such as methanogenesis by methanogens and acetate production by acetogens /Kotelnikova and Pedersen 1997/. There are also autotrophic iron- and sulphate-reducing bacteria that can use H_2 as an energy and electron source, concomitant with iron or sulphate reduction /Badziong and Thauer 1978/. The main products from biological anaerobic reactions are methane and acetate. If oxygen is available, H_2 is oxidised by some bacteria to water. H_2 can thereby contribute to the reduction of oxygen via microbial processes (see Section 5.7). The biological reactions remove H_2 from the geosphere.

Helium

After hydrogen, helium (He) is the most abundant element in the universe. He is mainly of primordial (solar) origin. The two naturally occurring isotopes are ^{3}He and ^{4}He. Nearly all terrestrial ^{4}He has been produced by radioactive decay of uranium and thorium over geological time. The most important source of ^{3}He is degassing of primordial volatiles from the Earth's interior. The ^{3}He/^{4}He ratio has been used to estimate groundwater residence times /Mahara et al. 2008/. He is lost from the atmosphere to space with a mean residence time of about 10^6 years. Canisters that fail may generate He from radioactive decay processes.

Chemical and biological reactions: He is an inert, non-toxic and non-flammable noble gas that does not participate in reactions.

Neon

Neon (Ne) is the geochemically most complex noble gas with three stable isotopes, ^{21}Ne, ^{22}Ne, ^{23}Ne and six short-lived radioactive isotopes. Ne has a primordial origin and is also formed via many different radioactive decay series. Its complex isotopic character makes Ne an important geochemical tracer.

Chemical and biological reactions: Ne is an inert, non-toxic and non-flammable noble gas that does not participate in reactions.

Argon

Argon (Ar) is the most abundant noble gas in the Earth's atmosphere and has three stable isotopes ^{36}Ar, ^{38}Ar and ^{40}Ar and twelve radioactive isotopes. Ar has a primordial origin and is also formed via many different radioactive decay series; the main source is decay of ^{40}K. Its complex isotopic character makes Ar an important geochemical tracer.

Chemical and biological reactions: Ar is an inert, non-toxic and non-flammable noble gas that does not participate in reactions.

Oxygen

Oxygen (O_2) is mainly found in the Earth's atmosphere. Its process of formation is by plants on the ground surface and by aquatic photosynthetic organisms. The process of O_2 formation requires light and includes the splitting of water to oxygen and protons in photosystem II with a concomitant oxidation of two oxygen atoms from water to O_2.

Chemical reactions: O_2 is highly reactive. It reacts, for example, with metals in the presence of an aqueous solution generally causing corrosion of the metal. O_2 can also react and oxidise different mineral components such as ferrous iron and sulphide.

Biological reactions: Several microorganisms have the ability to harvest energy by competing with spontaneous chemical processes in the oxidation of ferrous iron and sulphide with O_2. The microbial processes are generally adapted to be more rapid than the chemical process. Microorganisms can cause O_2 to react with several compounds that do not spontaneously oxidise chemically. The gases H_2, CO and CH_4 are all rapidly oxidised by different microorganisms /Chi Fru 2008, Pedersen et al. 2008/. In addition, microorganisms have the capacity to oxidise almost all natural organic compounds with O_2 /Madigan and Martinko 2006/. Microbial processes thereby can contribute significantly to the reduction of O_2 in the geosphere if the required reductants are present.

Nitrogen

Nitrogen (N_2) mainly has a primordial origin, meaning that this gas was aggregated during the accretion of the Earth, and N_2 have been degassing to the atmosphere through the geosphere since then. The source of N_2 in the atmosphere and geosphere is then degassing of primordial volatiles from the Earth's interior. Nitrogen is formed globally to a limited degree by biological reduction of nitrate, so called denitrification, under anaerobic conditions, such as those in marsh lands and shallow sea and lake sediments. Locally, the production of N_2 via denitrification can be large, provided that nitrate and a reducing component, generally organic carbon, are abundant.

Chemical reactions: There are no chemical reactions that involve N_2 in the geosphere under repository conditions.

Biological reactions: The fixation of N_2 by bacteria to ammonium is an anaerobic and energy demanding process. This is the only natural pathway for reduction of N_2 in the geosphere. Although the process is energy demanding, it is essential and supplies microorganisms with reduced nitrogen for biosynthetic pathways.

Carbon monoxide

Carbon monoxide (CO) is present as a minor constituent of the atmosphere, chiefly as a product of volcanic activity in deep layers. It occurs dissolved in molten volcanic rock at high pressures in the Earth's mantle. Natural and man-made fires and the burning of fossil fuels also add CO to the atmosphere. Deep groundwater always contains small amounts of dissolved carbon monoxide /Pedersen 2001, 2002/.

Chemical reactions: Although CO reacts with carbocations and carbanions, it is relatively unreactive toward organic compounds without the intervention of metal catalysts.

Biological reactions: CO is used as a source of carbon and energy by carboxydobacteria in aerobic environments and by methylotrophic and acetogenic bacteria in anaerobic environments such as the geosphere.

Carbon dioxide

Most of the world's carbon is contained in the geosphere, primarily in the form of carbonate rocks. Carbon dioxide (CO_2) is mainly contained in the oceans and to some extent in the atmosphere. The processes of formation of CO_2 and places of origin are a complex system, as it includes gas-water-mineral reactions, combustion of fossil and modern fuels, biological respiration of organic material and processes in the mantle. Inherent in this is that the places of origin are diverse as well.

Chemical reactions: Dissolved CO_2, is important to natural mineralogical processes that occur in the geosphere. When dissolved in water, the CO_2 molecule becomes hydrated to some extent, $CO_2(aq) + H_2O(l) \leftrightarrow H_2CO_3(aq)$, and dissociates to form carbonate and bicarbonate, rendering the groundwater acidic. These dissolved species can take part in a large number of chemical processes, for example the well-known dissolution-precipitation reaction of fracture-filling carbonates (calcite),

$$CO_2 + H_2O + CaCO_3\ (s) \leftrightarrow Ca^{2+} + 2HCO_3^-(aq)$$

and the weathering of minerals in the rock matrix (here exemplified by the weathering reaction of Ca-feldspar, anorthite, into kaolinite):

$$CaAl_2Si_2O_8(s) + 2H_2CO_3(aq) + H_2O \leftrightarrow Al_2Si_2O_5(OH)_4(s) + 2HCO_3^- + Ca^{2+}$$

Biological reactions: CO_2 is reduced to organic carbon by photosynthetic organisms and by chemolithotrophic bacteria. Photosynthesis is not a possible process in the geosphere. Chemolithotrophy includes methanogenesis and acetogenesis reducing CO_2 to methane and acetate, respectively.

Hydrogen sulphide

Hydrogen sulphide (H_2S) is a highly toxic and colourless gas that is very reactive and corrosive to metals. H_2S is formed from sulphate via thermogenic processes /Goldstein and Aizenshtat 1994, Cross et al. 2004/ in the crust and the mantle and via biological processes in anaerobic geosphere systems. H_2S dissolves readily and may dissociate in aqueous solutions to form HS^- and S^{2-}.

Chemical reactions: H_2S reacts with metal ions to form metal sulphides, thereby moving it out of solution. H_2S can increase the corrosion rates of iron and copper.

Biological reactions: Microorganisms can utilise H_2S as a source of energy in aerobic systems.

Methane

Methane (CH_4) forming processes comprise thermogenic, hydrolysis and biogenic reaction routes. Thermogenic generation occurs in deep crustal layers, whereas hydrolysis processes such as serpentinisation of ferrous materials can occur in both shallow and deep layers in the geosphere. The oxidation of ferrous material is coupled to the reduction of water to H_2, CO_2 to C or C to CH_4. Biological CH_4 production takes place in anaerobic systems with hydrogen and carbon dioxide, within the temperature limits of life, i.e. <113°C. CH_4 can also form by biological degradation of C-1 compounds such as methanol and formic acid and by degradation of acetate. Biological CH_4 formation then is restricted to the geosphere and the shallow part of deep layers.

Chemical reactions: There are no chemical reactions that involve CH_4 in the geosphere under repository conditions.

Biological reactions: Microorganisms can readily oxidise CH_4 with O_2. Intruding O_2 to the geosphere will be reduced with CH_4 if present /Chi Fru 2008/. Anaerobic CH_4 oxidation with sulphate /Boetius et al. 2000, Lösekann et al. 2007/ can occur in the geosphere.

C-2 and C-3 Hydrocarbons

Hydrocarbons are formed in parallel with thermogenic methane at depth. The presence of these gases together with methane is taken as an indication of thermogenic methane formation.

Chemical reactions: There are no chemical reactions that involve C-2 and C-3 hydrocarbons in the geosphere under repository conditions.

Biological reactions: There are no biological reactions that involve C-2 and C-3 hydrocarbons in the geosphere under repository conditions.

Dissolution of gases

The concentration of gases in groundwaters varies between sites and depending on the gas analysed /Pedersen 2001, 2002, Hallbeck and Pedersen 2008a/. Investigations at the Forsmark and Laxemar sites showed that nitrogen followed by helium are present in greatest amount with nitrogen and carbon dioxide being most common in the more shallow groundwaters and helium in the deeper parts of the system at Forsmark /Hallbeck and Pedersen 2008b/ and Laxemar /Hallbeck and Pedersen 2008c /. Methane has also been detected, but generally in small amounts. The total gas content measured was in the range 53–160 mL/L and generally increases with depth, but the waters are far from being oversaturated by gas. At some places, such as Olkiluoto in Finland, the methane concentration dominates at depth /Pedersen et al. 2008/. Gases from all sources may exist either as a free gas phase or dissolved in the local groundwater, and the extent to which a particular gas is in either state will vary with the conditions. There is intrinsic variation in the solubilities of the different gases (Table 5-10), but for all of them the solubility depends on both the gas pressure and temperature. The concentration of a gaseous species in an aqueous solution is, to a good approximation, directly proportional to the gas partial pressure (Henry's Law), and also decreases with an increase in temperature. Note that this means that, if a groundwater solution containing some dissolved gases comes into equilibrium with a free gas phase consisting of another gas, then some of the gases in solution will come out of solution until their partial pressures in the gas (which are initially zero) come into equilibrium with the solution concentrations. Bubbling a low solubility gas through a solution of other dissolved gases is a way of degassing the solution.

The dependence of solubility on pressure may be particularly significant in the context of a spent fuel repository because of the large variation in hydrostatic pressure between the repository and the surface (e.g. ~ 4 MPa at 400 m depth compared with 0.1 MPa at the surface, so the solubility would be 40 times higher at the repository depth compared with at the surface). As already mentioned, this means that dissolved gas may, depending on its concentration, come out of solution if the body of groundwater in which it is dissolved migrates from deep to shallow depths. An additional factor affecting the solubility of most gases is the salinity of the aqueous phase. In many cases, solubility is reduced by an increase in ionic strength (the salting-out effect), although this effect is generally smaller than that of temperature and total pressure.

When several gases are present in solution, a free gas phase will appear when the sum of the partial pressures of all the gases that are at equilibrium with the solution concentrations exceeds the hydrostatic pressure (strictly account also needs to be taken of the capillary pressure). The composition of the free gas phase at equilibrium is such that for each gas its partial pressure is in equilibrium with its dissolved concentration, that is, Henry's law is obeyed for each gaseous component:

$$c_i = H_i p_{gi}$$

where c_i, H_i, and p_{gi} are the concentration in the aqueous phase, the Henry's law coefficient, and the partial pressure in the gas phase of component i, and where the total gas pressure, p_g, is the sum of the partial pressures of the components in the gas phase:

$$p_g = \sum_i p_{gi}$$

5.10.2 Dependencies between process and geosphere variables

Table 5-11 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.10.7.

Table 5-11. Direct dependencies between the process "Formation/dissolution/reaction of gaseous species" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. The solubility of gases is temperature dependent. The reaction/formation of gases is temperature dependent as well.	All	Process neglected; no significant generation of gaseous species expected. Reactions including CO_2 and H_2S are included in the geochemical calculations.	Yes. But the effect of heat of solution/reaction is negligible.	All.	Process neglected; little heat effect from most gaseous processes except perhaps combustion.
Groundwater flow	Yes. Flowing groundwater carries dissolved gasses.	Excavation/ operation Temperate Periglacial	Process neglected; no significant generation of gaseous species expected. Reactions including CO_2 and H_2S are included in the geochemical calculations.	No, but indirectly if a sufficient amount of gaseous species are produced so that a gas phase is created. A trapped gas phase, the migration of gas bubbles, and instabilities in gas flow could affect groundwater flow.	All	Process not handled. Of little significance for groundwater flow.
		Glacial	Evaluation of the influence of inflow of oxygen with glacial melt waters. Reactions including CO_2 and H_2S are included in the geochemical calculations			

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Groundwater pressure	Yes. The solubility of gases is pressure dependent.	Excavation/ operation	Process neglected; small pressure effects.	Yes. The production of gases from corrosion, microbial processes and decomposition of construction and stray materials could raise groundwater pressure locally.	Excavation/ operation	Process neglected; little significance.
		Temperate Periglacial Glacial	Influence neglected; little significance.		Temperate Periglacial Glacial	The influence on groundwater pressure from the generation of gaseous species in the geosphere will be negligible.
Gas phase flow	Yes. A gas phase flow would influence the dissolution of the gaseous components in a water phase.	Excavation/ operation	Process neglected; little significance.	Yes. The generation of large amounts of gaseous species would increase the flow of the gas phase.	Excavation/ operation	Process neglected; little significance.
		Temperate	Influence neglected; little significance. Main gas would be hydrogen released from corrosion in the repository. This is considered when estimating bacterial sulphate reduction.		Temperate	Considered in scoping calculations of the capability of the geosphere to transport gas (see Section 3.2).
		Periglacial Glaciation	Process not handled; little significance.		Periglacial Glacial	Process not handled; little significance
Repository geometry	No. But indirectly by affecting the gas release to the geosphere.	–	–	No. No effect on geometry of deposition holes or tunnels is expected, but indirectly if a sufficient amount of gaseous species are produced so that a gas phase is created. Elevated gas pressure could disrupt the buffer or backfill.	–	–
Fracture geometry	No. But indirectly if a sufficient amount of gaseous species are produced so that a gas phase is created. Fracture geometry/ connectivity controls gas migration.	–	See Section 3.2.	No. But indirectly if a sufficient amount of gaseous species are produced so that a gas phase is created and if the gas pressure rises enough to dilate/induce fractures.	–	See Section 3.2.
Rock stresses	No. But indirectly through the effect of rock stresses on fracture properties/geometry.	–	–	No. No, but indirectly if a sufficient amount of gaseous species are produced so that a gas phase is created. An elevated gas pressure could affect rock stresses, but not expected to be significant in fractured rock.	All	See Section 3.2.
Matrix minerals	Yes. Weathering reactions will decrease the amount of dissolved O_2 and CO_2.	All	The geochemical models consider some reactions with carbon dioxide. Reactions of dissolved O_2 with matrix minerals are considered during glacial periods.	Yes. The dissolution of O_2 and CO_2 will induce reactions with minerals in the rock matrix. This process is however slow.	All	Neglected: observations of drillcores show that the matrix minerals are negligibly influence by reactions with gaseous species.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture minerals	Yes. Water-rock interactions will decrease the amount of dissolved O_2 and CO_2.	All	The geochemical models consider some reactions with carbon dioxide. Reactions of dissolved O_2 with fracture minerals are considered during glacial periods.	Yes. The dissolution of CH_4, O_2 or CO_2 will induce microbial processes or reactions with minerals in the fracture surface.	All	The fate of fracture filling minerals has not been evaluated directly in SR-Site. In geochemical calculations the amounts of minerals precipitating or dissolving have been calculated, and found to be of no significance.
Groundwater composition	Yes. Biological gas formation depends on groundwater chemistry and gas solubility depends on salinity.	Excavation/ operation	Process neglected; little significance.	Yes. Gaseous components are an integral part of groundwater composition.	Excavation/ operation	Process neglected; little significance.
		Temperate Periglacial	Process neglected; no significant generation of gaseous species expected. Reactions including CO_2 and H_2S are included in the geochemical calculations.		Temperate Periglacial	Reactions including CO_2 and H_2S are included in the geochemical calculations.
		Glacial	Considered in evaluation of oxygen consumption in glacial melt water. Reactions including CO_2 and H_2S are included in the geochemical calculations.		Glacial	Evaluation of oxygen consumption in glacial melt water. Reactions including CO_2 and H_2S are included in the geochemical calculations.
Gas composition	Yes. Dissolved gaseous species will depend on the composition of a gas phase, if present.	Excavation/ operation/	Process neglected; little significance.	Yes. The composition of a gas phase, if it exists and it is in equilibrium with groundwater, depends on the gaseous species in the groundwater. However the production of gaseous species in the geosphere will not be sufficient to influence a gas phase significantly.	Excavation/ operation	Process neglected; little significance
		Temperate	Neglected; main gas would be hydrogen released from corrosion in the repository. This is considered when estimating bacterial sulphate reduction.		Temperate Periglacial Glacial	Neglected; little significance.
		Periglacial Glacial	Neglected; little significance.			
Structural and stray materials	Yes. For example from iron and steel corrosion.	Excavation/ operation/	Process neglected; little significance.	No. But indirectly. For example CO_2 could dissolve in groundwater and react with concrete.	–	The composition of groundwater, including dissolved CO_2 has been used to evaluate grout degradation, see Section 5.8.
		Temperate Periglacial Glacial	Neglected; little significance. Main gas would be H_2 released from corrosion in the repository. This is considered when estimating bacterial sulphate reduction.			
Saturation	Yes. A gas phase would influence the dissolution of the gaseous components in a water phase.	Excavation/ operation	Process neglected; little significance.	Yes. But only if a sufficient amount of gaseous species are produced so that a gas phase is created: a free gas phase would create an unsaturated zone in the rock. However, this might be very localised.	All	Neglected; too small amounts of gaseous species are generated or consumed in the geosphere.
		Temperate	Neglected; little significance. Main gas would be H_2 released from corrosion in the repository. This is considered when estimating bacterial sulphate reduction			
		Periglacial Glacial	Process not handled: it is assumed that the rock volume is fully saturated.			

5.10.3 Boundary conditions

The state of gases (dissolved or free gas phase) in the geosphere and the significance of their reactions depends in part on their concentrations. For natural gases, their concentrations depend on exchange with atmospheric gases near the surface, the fluxes of gases from depth in the Earth's crust, reactions that will create or consume gases, and the transport of gases, either in solution in moving groundwater or as free gas phase. The release and transport of other substances in the groundwater may also have an impact on reactions involving gases. Some processes will release gaseous species and solutes from the engineered areas of the repository. These will add to the natural pool of gases and dissolved species. The release of gases, mainly H_2 from iron corrosion, from the repository is described in separate process description reports /SKB 2010d, e/.

Climate change, natural and anthropogenic, will lead to changes in the composition of infiltrating waters entering the geosphere, which in turn may lead to long-term changes in the gases present (see Section 5.10.6).

When the site is covered by an ice-sheet, melt-waters containing dissolved oxygen might intrude through conductive fractures if there are such fractures that are not sealed by frozen water (e.g. below warm-based ice-sheets). Bicarbonate-rich waters are expected to enter the geosphere in recharge regions in a temperate climate state (the conditions prevailing at present). Permafrost conditions will lead to complex changes in the deep groundwater flow regime. Where the surface is isolated from deep groundwaters by permafrost, the infiltration of meteoric waters will be substantially reduced; this includes reduction in the transport of dissolved atmospheric gases to depth. This is discussed in Section 3.1. From the point of view of the effect on the behaviour of gases, the important considerations are likely to be the effect of temperature and whether or not there will be an unsaturated zone between the deep water table and the base of the permafrost. However, the formation of an unsaturated zone beneath the permafrost is judged as rather unlikely, considering the climate conditions in Sweden; see the SR-Site Climate report /SKB 2010c/.The possible formation and decomposition of methane hydrates is discussed in Section 5.11.

5.10.4 Model studies/experimental studies

The dissolution of gases in groundwater is a well understood process that can be incorporated without great difficulty in numerical models of gas migration in the geosphere, if required. Repository-derived gases should in these respects behave in the same way as natural gases, except that the greater concentration of production locally means that there is a greater expectation that a free gas phase would be produced from repository derived gases than is the experience with natural gases.

5.10.5 Natural analogues/observations in nature

The presence and reactions of natural gases in the geosphere are well-established phenomena that are widely researched and documented /e.g. Apps and van de Kamp 1993/. The identification of natural analogues for the formation and reactions of gases produced in the repository has proved more elusive and none have yet been identified.

5.10.6 Time perspective

The formation and dissolution of gas concerns the whole period starting with repository construction until the isolating functions of the repository are no longer needed because of radioactive decay. Natural gases are likely to be supplied from the mantle during the timescales that need to be considered in a repository safety assessment. The gas generating potential of the cast iron in the spent fuel canisters and the predicted slow corrosion of this iron (should water contact the iron as a result of canister failure) and other iron and steel components in the repository mean also that gas could be produced in the repository for a very long period.

The timescales for the transfer of gases, mainly H_2 from iron and steel corrosion, from the repository tunnels and deposition holes into the geosphere are described in separate process description reports /SKB 2010d, e/. The timescales relating to gas migration in the geosphere are discussed in Section 3.2.6.

5.10.7 Handling in the safety assessment SR-Site

In near-surface waters, dissolved oxygen of atmospheric origin may be present. However, oxygen is highly reactive, in particular it oxidises dissolved Fe(II) and it reacts with Fe(II) minerals, and it provides the preferred electron acceptor for many microbes (see Section 5.7). This reactivity quickly removes the oxygen from groundwater and so it is not usually present by the time the groundwater has infiltrated to greater depths /Pedersen et al. 2008/, with the result that deep groundwater usually has reducing chemistry. During repository operations, there will be some desaturation of the rock around the repository cavities and in the rock close to the ground surface above the repository due to down-coning of the water table, although grouting will be used to reduce the effect. Aerated surface waters may also be drawn down to greater depths in the region of the repository. This means that oxygen will be drawn into regions of the geosphere in which conditions were previously reducing. This may introduce some changes in the state of minerals present and in microbial activity in this region of the geosphere during repository operations. However, once the repository is closed, these regions are expected to rapidly resaturate, and, once there is no continuing source of oxygen, the oxygen present will be rapidly consumed and anoxic conditions will be restored.

In general, the presence of natural gases, including their possible release as free gases and the redissolution of the free gases, is of no importance for the evolution of the repository. Possible radionuclide transport in a separate gas phase is dealt with in Section 6.2 and the possible effect of gas on water-borne radionuclide transport is dealt with in Section 6.1.

Dissolved methane and hydrogen may be involved in bacterial sulphate reduction, and the resulting sulphide could also affect the corrosion of the copper canister, but the mass transport of sulphide is highly dependent on water flow. The observed levels of sulphide in the groundwaters correspond to a steady state where the sulphate reduction process is ongoing, and the diffusive flows of methane and hydrogen assuming a deep crustal source are evaluated in SR-Site.

Excavation/operation

The processes are expected to have little significance. Desaturation of rock volumes adjacent to repository cavities will only add insignificant amounts of atmospheric gases as compared with the amounts of air entrapped in the buffer and backfill and can thus be neglected.

Temperate climate domain

Concentrations of dissolved natural gases are expected to remain substantially the same as those that exist now and therefore the analyses conducted for SR-Site are limited. Fluxes and maximum production rates of helium, methane and hydrogen are estimated based on the content of gas in the groundwaters at Forsmark and Laxemar /Delos et al. 2010/. In addition, the scoping calculations of gas generation and gas transport in the geosphere at constant temperature performed for SR-Can /Hartley et al. 2006a/ are applicable also for SR-Site. The rate of generation of repository gas is also included in these calculations. Constant salinity and corresponding gas solubilities are assumed in estimates of gas transport capacity in the geosphere.

Periglacial climate domain

During permafrost, natural gases that are continuously supplied from the mantle are likely to be transported by advection and or diffusion under the frozen rock, and be released at groundwater discharge points or diffuse through taliks. Potential impacts of the formation of methane hydrates are discussed in Section 5.11.

Glacial climate domain

In SR-Site, an evaluation is performed of the impact on repository safety of an intrusion of dissolved oxygen with melt waters during a glaciation. The evaluation includes reactions with rock matrix as well as microbially mediated processes, see Sections 5.5 and 5.7.

Earthquakes

Release of deep gases can be expected for short periods of times during earthquake events. Due to the short duration of such events the amounts of gaseous components released are expected to be negligibly small compared with the continuous flux and generation of gases during non-earthquake periods.

5.10.8 Uncertainties

Uncertainties in mechanistic understanding

Understanding of the partitioning of gas between dissolved and free gas phases is good.

The processes leading to the formation and distribution of natural gases are well characterised. As previously mentioned, the concentrations of dissolved gases in groundwaters vary greatly. This variation may be attributable to the varying sources of natural gases, the reactions in which they may be involved, and the way the dissolved gases are transported. However, the expected variability in natural gas concentrations at sites that could be chosen as a repository location is not thought to be significant for repository safety /Hallbeck and Pedersen 2008a, b/.

The main process, iron and steel corrosion, that leads to gas generation within the repository, is satisfactorily well characterised. Gas generation from corrosion in spent fuel canisters will only occur if a canister defect allows water intrusion into a canister. Uncertainties in the rate of water intrusion lead to uncertainties in the gas generation rate, but it is considered that it should be possible to adequately bound these rates for the purpose of a safety assessment. Although gas generation from spent fuel canisters and construction iron and steel is a near-field process, it provides a source term for gas in the geosphere.

Model simplification uncertainties in SR-Site

As far as the processes considered in this overall section are concerned, formation, dissolution, and reaction of gases in the geosphere, require only limited modelling. The formation and reaction of most natural gases is not modelled in SR-Site with a few exceptions; calculations involving the transport of helium, methane and hydrogen through the geosphere /Delos et al. 2010/, the possible formation of methane hydrates /Bahman et al. 2010/ and most importantly for the repository, the modelling of the effect of the enhanced infiltration of oxygenated glacial melt waters during glacial periods /Sidborn et al. 2010/. Model simplifications and uncertainties are evaluated in these underlying reports.

The partitioning of gases between dissolved and free gas phases is considered to establish the extent which a free gas phase will appear. This can be carried out in a simple way for the low solubility gases of interest using Henry's law. More exact formulations, including, for example, the effect of dissolved salts, would not change the conclusions for the safety case of a spent fuel repository.

Dissolved methane and hydrogen may participate in microbial processes. In particular, intrusion of sea water during the excavation and operation phases may induce reduction of sulphate to sulphide, if methane is present. Model uncertainties and simplifications in the evaluation of microbially mediated processes, which frequently involve the consumption or generation of gases, are discussed in Section 5.7.

Input data and data uncertainties in SR-Site

The coefficients that are needed to describe the partitioning of gas between dissolved and free gas phases are well known for pure water. Data on the effect of dissolved salts on gas solubilities appear less good, but the effect is not considered likely to be important.

Consideration of the effect of the impact on repository safety of an intrusion of dissolved oxygen with melt waters during a glaciation requires data on the rock and fracture mineralogy, thermodynamic data for the geochemical reactions in which the oxygen may be involved, and on the microbial processes which may consume the oxygen. Data uncertainties concerning reactions between groundwater and rock minerals are discussed in Section 5.5, and data uncertainties related to the evaluation of microbially-mediated processes are discussed in Section 5.7.

5.10.9 Adequacy of references supporting the handling in SR-Site

All references supporting the handling of gas generation and dilution processes have been published as peer review papers or are SKB reports that have undergone a documented factual review.

5.11 Methane hydrate formation

5.11.1 Overview/general description

Natural gas hydrates form under low-temperature, high-pressure conditions, both above and below the freezing point of water. They comprise solid crystalline compounds composed of molecules of natural gas trapped in cages of hydrogen-bonded water molecules (i.e. clathrates). Under proper conditions, the lattice is stabilised by van der Waals forces through the occupation of specific cavities within the lattice by certain types of guest molecules. The type of guest molecule(s) present determines which of the three known crystal structures the lattice assumes. Structure I is the most common form in a natural setting where methane is the main hydrate-forming gas, contributing to the structural stability by its small molecular size. Although this hydrate structure looks like ice and has a similar density, methane is concentrated to the extent that 1 m^3 of hydrate contains as much as 163 m^3 of methane at 1 atm and 273 K. Thus, the amount of energy in methane hydrate is much more than enough to support its own melting and combustion, and provide additional energy /Sloan 2004/.

In summary, four conditions are required to form hydrates /Sloan 2004/:

- low temperature (usually < 300 K),
- high pressure (> 38 bar hydrostatic pressure at 277 K),
- non-polar guest molecule smaller than 0.9 nm (methane), and
- presence of water.

The amount of solid hydrate formation will depend on the availability of the host water and the supply of methane molecules. Each hydrate-crystal structure devoid of methane is unstable and will collapse.

Knowledge of the stability conditions for methane hydrates is essential for understanding their role in geological processes. An important condition is the coexistence of methane hydrate with both liquid and vapour phases in a three-phase equilibrium. Figure 5-3 shows a methane-water mixture as a function of pressure (i.e. equivalent depth assuming a hydrostatic pressure gradient of 10^4 Pa m^{-1}) and temperature (K). Methane hydrate is stable when the temperature is less than or equal to $T_3(P)$; when less than $T_3(P)$ the hydrate phase coexists with either the liquid or vapour phases, depending on their relative abundances.

The role of temperature, when methane hydrate coexists with liquid solution, was underlined by /Zatsepina and Buffett 1997/, see Figure 5-4. The solid line represents the solubility of methane in pure water. An increase in the temperature of a mixture of methane and water above $T_3(P)$ lowers the methane solubility and, conversely, the opposite occurs at temperatures below $T_3(P)$ when hydrate is present. The latter has two important implications: a) cooling causes formation of methane hydrate, since gas in excess of the solubility is removed from the liquid phase, and b) the stability temperature achieved by methane hydrate depends on the pressure and concentration of dissolved gas.

Under permafrost conditions, where temperatures are below 0°C, the methane hydrate coexists with the vapour phase (Figure 5-3). In a two-phase equilibrium, ice cannot coexist with the methane hydrate because the concentration of gas in the ice is too low. Ice should convert to hydrate in the presence of methane, but the low diffusivity of gas in ice may allow the persistence of ice under non-equilibrium conditions /Sloan 2004/.

Figure 5-5 shows that methane hydrate is stable over a greater thickness of bedrock in areas where low temperature permafrost conditions prevail and the thermal gradient is small. Methane hydrate is generally unstable in the uppermost approximately 200 m or in areas where the permafrost depth is less than 200 m. The shaded area to the left of the methane hydrate stability curve represents conditions for methane hydrate stability. Methane hydrate is stable when the temperature for a

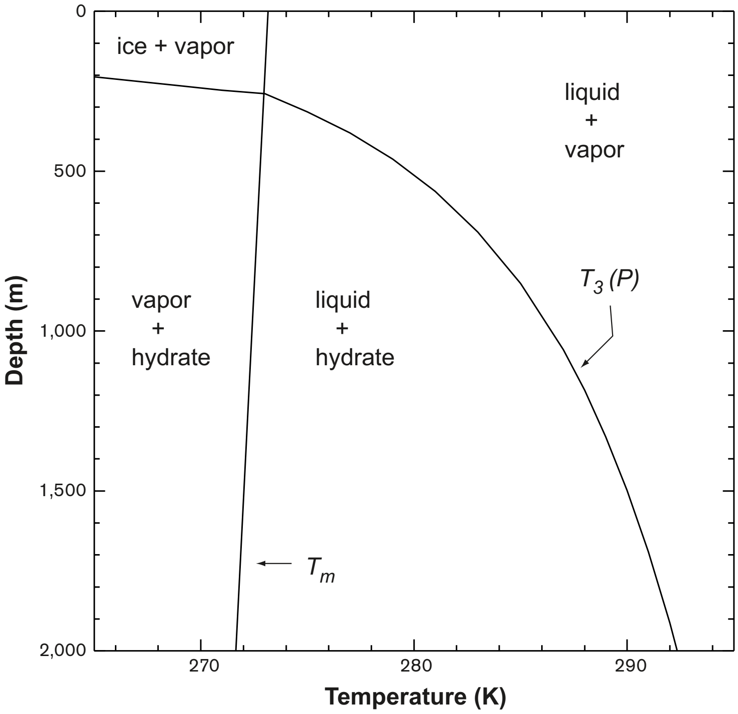

Figure 5-3. *Phase diagram for a methane-water mixture as a function of depth and temperature. Temperature $T_3(P)$ bounds the region where hydrate is stable and T_m is the melting temperature of pure water; after /Buffett 2000/.*

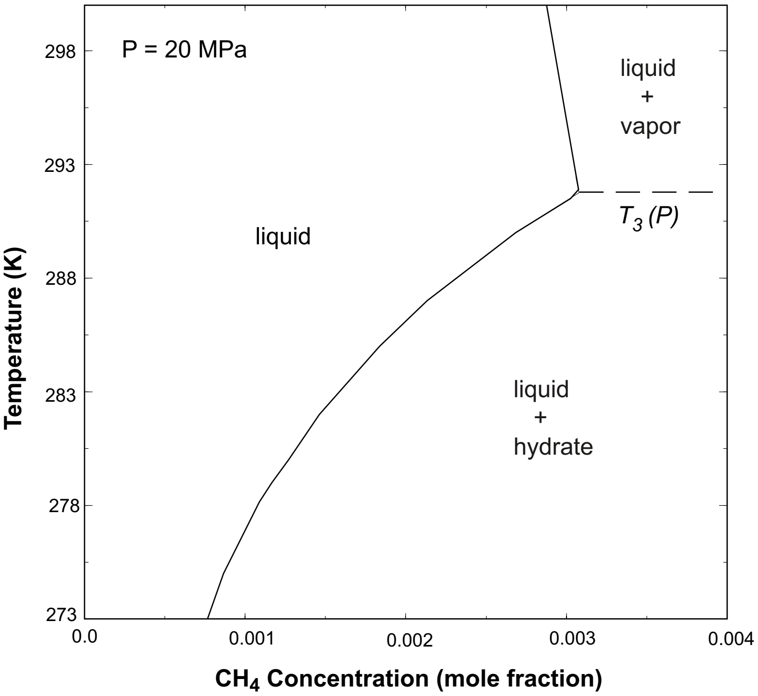

Figure 5-4. *Phase diagram for a methane-water mixture as a function of temperature and gas concentration. The solid line represents the solubility of gas in equilibrium with either vapour or hydrate; after /Buffett 2000/.*

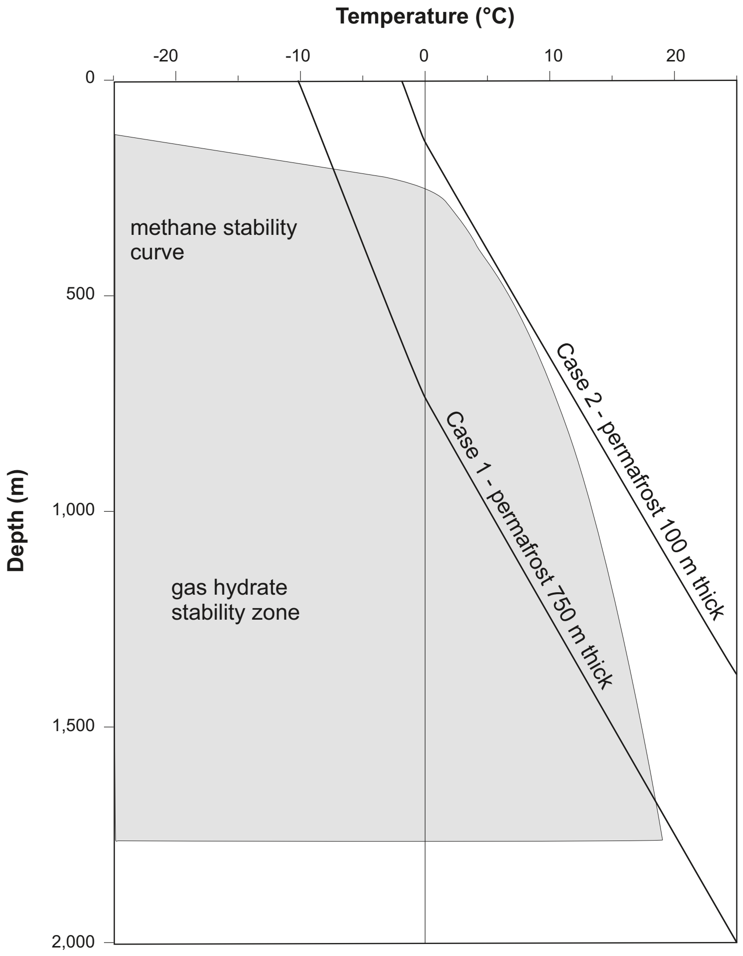

Figure 5-5. *Theoretical subsurface temperature profiles (geothermal gradient = 20°C/km) typical of the Canadian bedrock permafrost region superimposed on the methane hydrate stability curve (cf. Figure 5-3); after /Smith 2001/.*

given depth occurs within this shaded area. The methane hydrate stability zone is more extensive at thick permafrost locations. In case (1), the methane hydrate stability zone extends to depths around 1,650 m where permafrost is 750 m thick. In case (2), the methane hydrate is unstable where the permafrost is only 100 m thick /Smith 2001/. Below the base of the methane hydrate stability zone, liquid water and methane gas bubbles would be expected to occur.

An additional factor which may influence methane hydrate stability is the presence of dissolved salts (e.g. presence of saline groundwaters). Dissolved salts lower the equilibrium temperature $T_3(P)$ by 1–2°C over a range of salinity characteristic of seafloor sediments. Thermodynamically, the main effect on the three phase equilibrium (cf. Figure 5-3) is to lower the free energy of the water molecules in the liquid, thus inhibiting the formation of the methane hydrate. Salts also increase the free energy of gas molecules in solution, but this has little effect on hydrate stability. However, in the absence of a vapour phase, salt continues to lower the free energy of the water molecules in solution resulting in a 4–5% reduction in methane solubility in the presence of hydrate. Less gas in solution is required to stabilise the methane hydrate, thus the presence of salts actually increases hydrate formation from water in the absence of a gas phase /Buffet 2000/.

Temperature increases or pressure decreases leading to permafrost decay will result in changes in the thickness of the gas hydrate stability zone. Where dissociation of the solid methane ice phase to water and methane gas occurs, there will be a volume change that may affect the rock, especially if large quantities are transformed at the same time. In the Fennoscandian context, dissociation will begin once the temperature increase under the warm-based ice mass (or in the atmosphere if no ice mass is present) penetrates through the top 200 m of the permafrost. Evidence of methane release is seen in ice cores from Antarctica. These show a decrease in atmospheric methane concentration during the glacial period followed by a rapid increase in methane at the onset of interstadial warming /Stauffer et al. 1998/.

The permafrost horizon may reach depths of 150 m or more. For example, in northern Canada permafrost presently exists down to depths between 400–600 m at the Lupin Mine locality /Ruskeeniemi et al. 2002, 2004/. According to /Tarasov and Peltier 2007/, there is an 80% probability that permafrost completely melted at this site during the last glacial maximum, although relict permafrost cannot be completely ruled out. Permafrost at Lupin therefore likely started to form following rapid retreat of the ice sheet at the beginning of the last periglacial period, some 8,000 to 6,000 years ago /Smith 2001/. The development of permafrost in Sweden is described in the SR-Site Climate report /SKB 2010c/.

At or near the bedrock surface, the source of methane is usually biogenic in origin. At deeper levels it can be assumed that it is only in a few highly conductive fracture systems that an upward transport and enrichment of methane, mostly abiogenic in origin, is possible. Methane hydrate can therefore form in reasonable quantities in the upper part of the bedrock with the onset of permafrost, and continue to form at increasing depth during permafrost conditions, although its formation will be restricted to the conductive fracture systems. In areas affected by permafrost, the perennially frozen horizon could effectively form an impervious cap, which may serve to trap, concentrate and convert the upward transported methane gas (mainly abiogenic) into hydrates. In nature, methane hydrate has been observed in marine sediments and underneath permafrost (see below).

Repository implications

An eventual build-up of methane gas hydrates above a repository for nuclear spent fuel may give rise to some safety concerns during the expected lifespan of the repository. These include:

1. Important hydrogeological and geochemical implications of methane hydrate formation. During permafrost there is the potential for sealing of porosity and fracture space, thus reducing bedrock permeability. The groundwater chemistry can be affected by the freeze-out of salts well below the extent of the permafrost, to the base of hydrate formation, because methane hydrates are stable well beneath the permafrost base.
2. When subsequent dissociation of the solid methane hydrate phase to water/ice and methane gas release (e.g. during warm periods), there will be a volume change that may affect the rock, especially if large quantities are dissociated in a short period of time in a confined area. It could be speculated that this may lead to a reduction in the strength of the bedrock hosting the repository mass by inducing cracks or reactivating existing fractures, and therefore potentially increasing the groundwater flow in the upper part of the repository bedrock.
3. In the context of a repository engineered barrier system, the melting of gas hydrates, as well as the melting of permafrost, could result in a volume of rock where the fracture groundwaters are poor in dissolved salts. It could be speculated that these groundwaters could affect the long-term stability of the bentonite buffer material.

At a repository location, there will be three sources of temperature increase: a) heat from the spent fuel packages, b) heat from climate changes, and c) geothermal heat. During a glaciation, a sub-glacial permafrost horizon may begin to melt and decay when an ice sheet has formed on the land surface. What the consequences are for repository safety when dissociation occurs are difficult to foresee, since it will depend on the extent and depth of the permafrost horizon. Some fractured block masses at the surface in Fennoscandia have been interpreted to have resulted from spontaneous methane hydrate dissociation /Sjöberg 1994/, but any evidence for such events deeper down in the bedrock has not yet been recorded.

In the absence of permafrost, it is generally considered unlikely that methane hydrate formation will occur in a deep repository on a scale of importance to the safety of the repository. In order for this to happen, methane must be present in relatively large amounts at a depth of 500 m in order to combine with water and form methane ice. The solubility of methane is 4 g/L at normal pressure and 20°C. To occur in the gas phase at repository level at the hydrostatic pressures prevailing there, a concentration of over 200 g/L of dissolved methane is needed, i.e. very high concentrations of dissolved gases. Actual concentrations of dissolved gas are always much lower /Hermansson et al. 1991a, b/.

5.11.2 Dependencies between process and geosphere variables

Table 5-12 shows how the process is influenced by, and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.11.7.

Table 5-12. Direct dependencies between the process "Methane hydrate formation" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes.	Periglacial Glacial	Generic calculations to assess the possibility of methane hydrate formation.	Yes. By latent heat of melting/freezing.	Periglacial Glacial	The influence of methane hydrate formation on the temperature of the rock has not been evaluated but it should be similar to that of ice formation see Section 2.2.
Groundwater flow	No. But indirectly by advection of methane.	–	–	No. But indirectly by changing fracture geometries.	–	–
Groundwater pressure	Yes.	Periglacial Glacial	Generic calculations to assess the possibility of methane hydrate formation.	Yes. By expansion of the ice.	Periglacial Glacial	The influence of methane hydrate formation on groundwater pressure has not been evaluated but it should be similar to that of ice formation see Section 2.2.
Gas phase flow	No. But indirectly by bringing methane in contact with ice.	–	–	No. But indirectly by changing fracture geometries.	–	–
Repository geometry	No. But indirectly by the heat flow from the repository, and by affecting the flow of methane.	–		No.	–	–
Fracture geometry	Yes. Location of hydrate formation and also through the adsorptive capacity of the porous medium. In addition, influences the overall pathway for methane transport.	Periglacial Glacial	The influence of fracture geometry has been evaluated in SR-Site. The generic model calculations indicate that the formation of methane hydrates may be disregarded.	Yes. By affecting porosity, and potentially methane hydrate may open up or expand fractures.	Periglacial Glacial	Neglected: of little significance. See also Section 2.2.
Rock stresses	No. But indirectly by affecting porosity.	–	–	No. But indirectly through fracture geometry.	–	–
Matrix minerals	No. But, indirectly through thermal properties of rock matrix.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture minerals	No. The adsorption of water molecules on mineral surfaces decreases the freezing temperature. However, this effect should be similar for different types of minerals.	–	–	No.	–	–
Groundwater composition	Yes. The freezing temperature of water to ice decreases as the salt content increases.	Periglacial Glacial	Generic calculations to assess the possibility of methane hydrate formation.	Yes. The formation of methane hydrates would deplete surrounding groundwater from methane; and salt exclusion may occur.	Periglacial Glacial	Should be similar to the formation of ice: see Section 2.2.
Gas composition	Yes.	Periglacial Glacial	Generic calculations to assess the possibility of methane hydrate formation.	Yes. Removal of methane.	Periglacial Glacial	Neglected: The generic calculations indicate that methane hydrate formation may be disregarded, and no gas phase is expected in the rock volume at the site.
Structural and stray materials	No. But, indirectly through their thermal properties and changes in groundwater composition.	–	–	No. Provided that freezing does not occur at repository depth.	–	–
Saturation	Yes.	Periglacial Glacial	Neglected; saturated conditions in the bedrock is assumed.	Yes. The dissociation of large amounts of hydrate might result in large quantities of gas resulting in localised and short-lived unsaturation of the rock.	Periglacial Glacial	Neglected; saturated conditions in the bedrock is assumed.

5.11.3 Boundary conditions

The exchanges of methane gas and of heat with the biosphere and with deep parts of the geosphere comprise the boundary conditions for the formation or dissociation of methane hydrates. Climate change will lead to changes in surface temperatures and heat-transfer parameters, which in turn may lead to the formation and melting of methane hydrates over long periods of time.

5.11.4 Model studies/experimental studies

Because of the economic importance of gas hydrates as a future energy source, there is an abundance of experimental and model data published in the open literature, for example, comparing laboratory-derived synthetic clathrate hydrates with those naturally formed /Stern et al. 2004/. Understanding the alteration evolution of naturally occurring hydrates may help to unravel their *in situ* state or growth processes. Other laboratory studies referred to above /Circone et al. 2004/ addressed the effect of elevated methane pressure on methane hydrate dissociation.

Modelling simulations were carried out to assess the risk of methane hydrate formation during future permafrost conditions at candidate sites in Sweden and Finland /Bahman et al. 2010/. The main conclusion is that the risk of hydrate formation is unlikely at the reported methane concentrations and water salinities.

5.11.5 Natural analogues/observations in nature

Several sites presently under permafrost conditions have been, or, are in the process of being investigated. These include crystalline rocks in Canada, e.g. / Ruskeeniemi et al. 2002, 2004, Stotler et al. 2009, Holden et al. 2009/, deep sedimentary rocks in Russia, e.g. /Alexeev and Alexeeva 2003/, and sea sediments in Canada, e.g. /Dallimore and Collett 1995, 1999, Clark et al. 1999/. Of the many observations documented, the Mallik sea sediments in the MacKenzie Delta, Northwest Territories, Canada, represent the first concerted effort to study the occurrence of natural gas hydrates in a permafrost environment. The objectives were to obtain geological, geophysical and geochemical data of the Mallik gas hydrate field and to perform production testing of a concentrated gas hydrate reservoir. The physical behaviour of the hydrate deposits was monitored after depressurisation and thermal stimulation. Gas-hydrate-bearing core samples were collected and down-hole geophysical logging was performed. In parallel, detailed laboratory experiments (see above) were conducted providing greater physicochemical understanding of the formation, stability and ultimate dissociation of these hydrate phases under similar permafrost conditions to those expected during future climate change in Fennoscandia.

No methane hydrates have been found during the Lupin Mine studies, but indicators of their past presence were noted by /Stotler et al. 2009/. This included the identification of possible areas beneath the permafrost layer where mine-induced depressurisation is thought to have resulted in melting of methane hydrates, contributing to the dilution observed in some subpermafrost groundwaters.

5.11.6 Time perspective

Methane hydrates may only form during periods of permafrost or glaciation.

5.11.7 Handling in the safety assessment SR-Site

Excavation/operation period and temperate climate domain

Methane hydrate formation cannot take place during these periods at a repository site.

Periglacial- and glacial climate domains

Present-day knowledge indicates that the formation of substantial amounts of methane hydrates can have consequences for the hydrological properties of the rock around the repository even if permafrost does not reach repository depth. Modelling simulations have been carried out to assess the risk of methane hydrate formation during future permafrost conditions at candidate sites in Sweden and Finland. The main conclusion is that hydrate formation is unlikely at the reported methane concentrations and water salinities /Bahman et al. 2010/. Therefore, no further analyses of the consequences of methane hydrates are conducted for SR-Site.

Earthquakes

Continental-slope failures of sediments containing large methane hydrate occurrences have led to large scale releases of methane that have been observed in ice-core atmospheric records of the Pleistocene. Some continental-slope failures /e.g. Bugge et al. 1987/ are believed to have been triggered by the lowering of the sea level resulting in a reduction of hydrostatic pressure and a corresponding destabilisation of the methane hydrates /Maslin et al. 2004/. Earthquake activity is also an important and common mechanism for methane hydrate release along subduction zones /e.g. Jahren et al. 2005/. Theoretically, therefore, in a Fennoscandian context, earthquake activity of adequate strength occurring in a fractured crystalline rock repository environment could destabilise any accumulated methane hydrate. However, this is unlikely due to the small amounts of methane hydrate expected to form /Bahman et al. 2010/, and the rarity of substantial tectonic activity in Fennoscandian Shield.

5.11.8 Uncertainties

Uncertainties in mechanistic understanding

Methane ice formation is a physically well understood process.

Model simplification uncertainties in SR-Site

Not relevant.

Input data and data uncertainties in SR-Site

Not relevant.

5.11.9 Adequacy of references supporting the handling in SR-Site

There is a wealth of literature available on methane hydrates because of their potential for a future energy source. Much of the methane hydrate occurrences of economic potential tend to be mainly associated with shallow sea environments in polar regions, and major studies have been conducted in the Mallik sea sediments in the MacKenzie Delta, Northwest Territories, Canada. This is referenced above. In contrast, crystalline rock environments are economically of less interest and therefore there are few sources of literature available. The literature cited above covers the most relevant published information on crystalline occurrences. The report /Bahman et al. 2010/, supporting the neglect of further analyses of the consequences of methane hydrates in SR-Site, is a SKB report that has undergone a documented factual- and quality review.

5.12 Salt exclusion

5.12.1 Overview/general description

When water freezes slowly, the solutes present in the water will not be incorporated in the crystal lattice of the ice. This slow and continuous freezing process will accompany the onset and evolution of permafrost conditions at the surface and in the bedrock in advance of ice cover during future glaciation events. During this process, salts that have been present in the surface waters and groundwaters will tend to accumulate at the propagating freeze-out front. However, it should be noted that this front is not necessarily sharp, because freezing will take place over a range of temperatures, depending on the salinity and on the ratio between ‘free’ and tightly adsorbed water molecules, cf. Section 2.2.1. The freezing process could, if repeated a number of times, give rise to a boundary between fresh and saline water at the depth to which the perennially frozen front had reached. Depending on the geometry of the groundwater-containing fracture system, pockets of saline, unfrozen waters could also become confined within the permafrost.

Assuming initially saline water, either surface marine in origin or the product of mixing and/or water/rock interaction in the bedrock, this freeze-out process may produce residual waters of greater salinity, or in extreme cases even of brine character (> 100 g/L TDS), and rich in sulphate. One might speculate that the subsequent penetration of such a potential source of sulphate to repository depths might promote canister corrosion through the production of sulphide from microbial activity (i.e. sulphate-reducing bacteria) if large amounts of methane or organic matter would also become available. In addition, the presence of brine can lead to deterioration of the bentonite buffer material.

The freeze-out process has been simulated in the laboratory using seawater and temperatures down to –14°C /Thompson and Nelson 1956, see below/. This resulted in a concentration factor of about 5; in the residual brine portion the sulphate is in the form of mirabilite ($Na_2SO_4 \cdot 10H_2O$) supplemented by hydrohalite ($NaCl \cdot 2H_2O$). Freeze-out processes have been used to explain some of the saline lake occurrences in Antarctica, where it was referred to as ‘freeze-drying’ or ‘freeze concentration’ /Matsubaya et al. 1979, Burton 1981/. Since then, the contribution of a freeze-out process has been discussed in relation to the deep Canadian Shield brines, e.g. /Herut et al. 1990, Bottomley et al. 1994, 1999, Starinsky and Katz 2002/, where the chemistry of the brines may reflect both evaporative and cryogenic processes. In the context of Fennoscandia, /Bein and Arad 1992/ proposed that bedrock saline groundwaters present in coastal areas of the Baltic Sea are the result of the freezing of seawater which may have occurred just prior to the over-riding of a marine body by a glacier. The coastal areas of Hudson Bay in Canada may have been similarly affected.

In parts of northern Canada, permafrost presently exists to between 400–600 m depth /Ruskeeniemi et al. 2002, 2004, Holden et al. 2009/, and most is thought to date back to the last Pleistocene glaciation /Tarasov and Peltier 2007/. However, such deep permafrost is only likely to develop in cold areas that are typically not covered by ice sheets during long periods of glacial cycles. In Sweden, ice sheets are present for parts of the glacial cycles, thereby limiting the development of deep permafrost, see SR-Site Climate report /SKB 2010c/. Of course this does not preclude freeze-out processes having influenced the Baltic region, but the extent can be debated. The difficulty is estimating the spatial extent of the resulting brines, both laterally and vertically into the bedrock. Surface-derived brines from seawater freezing would, through density differences, be expected to penetrate into the bedrock until equilibration occurred with existing brines. This would have to be followed by lateral movement towards the mainland, a mechanism difficult to envisage hydrogeologically /Gascoyne 2000/. In contrast, permafrost formation in the bedrock is *in situ* and the slowly propagating freeze-out front would push the concentrating brines to depths which so far can only be estimated through model calculations.

Of course, under surface and near-surface bedrock conditions where fresh or weakly brackish meteoric waters dominate, no great changes are expected in the salinity of the groundwater during permafrost. Salt exclusion due to freezing at shallow depths could increase the salinity of the groundwater, but because the salinity of the groundwater is expected to be low before the onset of permafrost, the effect of salt exclusion can probably be considered negligible. Furthermore, generic simulations carried out by /Vidstrand et al. 2006/ suggest that a regional groundwater flow beneath a permafrost layer would cause a “flushing” of the rejected salt and hence dilute the salinity. With sufficient salinity, one of the main geochemical indicators to trace the presence of permafrost freeze-out brines in present-day groundwaters would be the preservation of sulphate-rich groundwaters resulting from the dissolution of mirabilite. Other residual fluid indicators in groundwaters include ^{11}B, ^{18}O and ^{2}H (and possibly ^{37}Cl) from freeze-out fractionation /e.g. Ruskeeniemi et al. 2004, Zhang et al. 2006, Casanova et al. 2004/. Unfortunately, because of flushing out and mixing of the groundwaters close to the Baltic Shield coastline following ice-sheet decay and isostatic recovery, many of the freeze-out brine signatures have either been removed or diluted, or may have migrated to depth and mixed with existing brine compositions.

The best possibilities to specifically detect the effects of permafrost activity include a mineralogical signature, for example, the formation of heavy δ^{13}C calcites /Clark and Lauriol 1992/, or finding by chance a preserved pocket/lens of brine in low permeable fractured parts of the bedrock (i.e. dead-end pathways and microfractures) or, more likely, present in the rock matrix porewater /Laaksoharju et al. 2009a, Waber et al. 2009a/.

5.12.2 Dependencies between process and geosphere variables

Table 5-13 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.12.7.

Table 5-13. Direct dependencies between the process “Salt exclusion” and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. The amount and composition of the saline water is temperature-dependent.	Periglacial Glacial	Simplified and pessimistic assumption regarding the quantity of out-frozen salt (see Section 5.12.8).	No.	–	–
Groundwater flow	No. Although groundwater flow under the permafrost layer may remove the accumulating salts.	–	–	Yes. Saline waters have higher density and will influence groundwater flow by gravitational effects.	Periglacial Glacial	Included in a generic model of groundwater flow under permafrost, see Section 3.1.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**	**Influence present? (Yes/No? Description)**	**Time period/ Climate domain**	**Handling of influence (How/If not – Why)**
Groundwater pressure	Yes. Pressure affects the freezing temperature of water, and thus the exclusion of salts.	Periglacial Glacial	Simplified and pessimistic assumption regarding the quantity of out-frozen salt (see Section 5.12.8).	No.	–	–
Gas phase flow	No. Only by the temperature of the gas phase.	–	–	No.	–	–
Repository geometry	No.	–	–	No.	–	–
Fracture geometry	Yes. Fracture geometry influences the overall pathway for the freeze-out front and the accumulating salts.	Periglacial Glacial	Included in a generic model of groundwater flow under permafrost, see Section 3.1.	No.	–	–
Rock stresses	No. Only indirectly if they affect fracture geometry.	–	–	No.	–	–
Matrix minerals	No. There is no evidence so far to indicate that the freeze-out front passes through the rock matrix.	–	–	No. The matrix simply undergoes in situ freezing.	–	–
Fracture minerals	No. The adsorption of water molecules on mineral surfaces decreases the freezing temperature. However, this effect should be similar for different types of minerals.	–	–	No. But indirectly through groundwater composition since production of saline waters may lead to precipitation of new phases.	–	–
Groundwater composition	Yes. Affects the salts that may be frozen out.	Periglacial Glacial	Generic model of groundwater flow under permafrost assumes present day depth profile for salinity.	Yes.	Periglacial Glacial	Groundwater salinities evaluated through a generic model of density-driven flow under permafrost, see Section 3.1.
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No.	–	–	Yes. Potentially detrimental – chemical brine-induced degradation of cement and metal corrosion.	Periglacial Glacial	Degradation of grout not evaluated for permafrost conditions in SR-Site, see Section 5.8.
Saturation	Yes.	Periglacial Glacial	Influence not considered; saturated conditions assumed.	No.	–	–

5.12.3 Boundary conditions

The compositions of the waters and the temperature at the surface comprise the boundary conditions for the freezing of the surface and near-surface groundwaters with resulting salt exclusion.

Climate change will lead to changes in surface temperatures and water compositions, which in turn may lead to the formation of ice over long periods of time with the consequent exclusion of salts.

5.12.4 Model studies/experimental studies

The freeze-out hypothesis is largely based on laboratory experiments related to sea water freezing, where, for example, /Nelson and Thompson 1954/ were able to distinguish between the products of evaporation and freezing. The solid products from evaporation consisted of halite with subsidiary gypsum, and from freezing, hydrahalite and mirabilite. The most important difference during freezing is the removal of the SO_4^{2-} ion in mirabilite ($Na_2SO_4 \cdot 10H_2O$). However /Marion et al. 1999/, based on theoretical model and experimental evidence, demonstrated that gypsum also can precipitate spontaneously after mirabilite and at lower temperatures during sea water freezing, arguing that its inclusion is the most thermodynamically favoured pathway and close to that earlier proposed by /Gitterman 1937/. Moreover, from a theoretical point of view, depending on the Na/Ca ratio of the groundwater type present prior to permafrost activity, gypsum may be the first precipitated phase during freezing instead of mirabilite.

The 'freeze-out' concept, as described and discussed by /Bein and Arad 1992/, assumes that the formation of permafrost in a brackish lake or a restricted coastal sea environment (e.g. similar to that of the Baltic Sea or Hudson Bay in Canada) produced a layer of highly concentrated salinity ahead of the advancing freezing front. Since this saline water would be of high density, it subsequently would sink to lower depths (i.e. density driven intrusion), would avoid dilution by oceanic water, and potentially penetrate into the bedrock where it would eventually mix with formational groundwaters until the density of the mixtures became similar to that of the existing groundwater at the current elevation.

Where the bedrock is not covered by brackish lake or restricted sea water, similar freeze-out processes may occur in the bedrock on a much smaller scale within the hydraulically active fractures and fracture zones, again resulting in formation of a higher density saline component in the residual fluids. The incremental downward propagation of the freeze-out front will eventually cease due to increased salinity, increased temperature, and a decrease in transmissivity that will hinder potential pathways for the residual fluids.

Recent work /Ruskeeniemi et al. 2004, Zhang and Frape 2003, Zhang et al. 2006/ describes freezing experiments using waters other than seawater; a $Na\text{-}SO_4$ groundwater from Palmottu, Finland and a Ca-Cl groundwater from Sudbury, Canada. In common with the seawater experiments, with progressive freezing all ions in the residual solutions showed an increasing trend towards greater concentrations. In addition, $\delta^{18}O$ and $\delta^{2}H$ became increasingly depleted. Compared with the Baltic and Canadian Shield brines, the resulting residual solutions from the freeze-out experiments generally plot at a higher sulphate concentration for a specific chloride concentration. Two mechanisms occurring *in situ* were invoked to explain this disparity: a) sulphate was removed as mirabilite, and b) sulphate was removed by microbial reduction to sulphide. Both processes are considered possible under permafrost conditions.

5.12.5 Natural analogues/observations in nature

Many studies have been reported from sites throughout the Canadian Shield (mostly deep mine localities) and these are adequately referenced in /Bottomley et al. 1999/ and /Gascoyne 2000/. Evidence for permafrost in crystalline rock environments was specifically addressed in the Palmottu natural analogue study /Blomqvist et al. 2000/ and since then has been a focus in studies of the Lupin Mine, Canada /Ruskeeniemi et al. 2002, 2004, Stotler et al. 2009/, High Lake, Canada /Holden et al. 2009/ and in the various site characterisation investigations being carried out in Sweden and Finland, e.g. /Laaksoharju et al. 2008b, 2009a/. The large number of methane hydrate studies have also referred to the presence of residual fluids from ion exclusion during ice formation at the base of the permafrost layer /Torres et al. 2009/.

The Lupin Mine studies have now been concluded, and while freezing processes are inferred to have occurred (e.g. the possibility of methane hydrate formation), the degree to which the freezing has modified the chemistry of the site has been difficult to quantify /Stotler et al. 2009/. This difficulty has been compounded by the nature of the site, where there is widespread contamination due to long-term mining activities and also mixing of different groundwater types beneath the permafrost layer.

Mixing of different groundwater types has also plagued interpretation of the hydrochemical data from the Swedish sites, but some indication of freezing processes may have been preserved, especially at the Laxemar site /Laaksoharju et al. 2008b, 2009a/. The isotopes of oxygen, boron and chlorine can be sensitive to freeze-out conditions, either becoming enriched in the ice phase (^{18}O and ^{37}Cl) or in the residual fluid phase (^{11}B). These isotopes have been investigated in the Laxemar groundwaters, in particular the brackish glacial type, which mostly occurs at intermediate depths (about 300–600 m) and appears to have been reasonably well preserved in bedrock that shows a decrease in hydraulic conductivity with increasing depth. The data show enrichment in ^{11}B which has accumulated in most of these groundwaters and may be a result of freeze-out processes. In addition, the distribution of $\delta^{37}Cl$ shows a weak correlation between increasing enrichment of ^{37}Cl corresponding to a depletion of $\delta^{11}B$ in the same groundwaters, supporting also a possible freezing effect. Furthermore, two samples in particular show enriched ^{11}B together with depleted ^{18}O and possibly depleted ^{37}Cl, which may suggest a modification of the isotope systems related to freeze-out processes.

A number of porewater samples from depth intervals of about 430–550 m and 620–750 m at Laxemar show accumulated Na-Ca-SO_4 compositions. The origin of this sulphate is not clear, but possible sources are dissolution of gypsum and/or modifications induced by freezing processes.

In conclusion, whilst there is some support for freeze-out processes having occurred at Laxemar (less so at Forsmark), the degree to which the freezing has modified the chemistry of groundwaters, in common with the Lupin Mine studies, has been impossible to quantify.

5.12.6 Time perspective

Salt exclusion due to freezing may only occur under periods of permafrost or glaciation.

5.12.7 Handling in the safety assessment SR-Site

Excavation/operation period and temperate climate domain

Salt exclusion by freezing will not take place during these periods.

Periglacial- and glacial climate domains

Generic calculations showing the evolution of saline waters under permafrost are used to evaluate the possible impact at repository level /Hartikainen et al. 2010, Vidstrand et al. 2010a, b/. This generic model shows that saline waters generated from freezing will have higher densities than the original groundwaters and they are, therefore, expected to move downwards, especially in highly conductive fractures. In the less permeable rock mass, permafrost is expected to advance faster than the movement of salts and a salt front is not formed /Vidstrand et al. 2006/.

Earthquakes

No relation between earthquakes and salt exclusion by freezing has been identified.

5.12.8 Uncertainties

Uncertainties in mechanistic understanding

The process of salt exclusion due to freezing is well understood. There is some uncertainty concerning the extent to which permafrost has influenced the salinity of groundwaters found at depth at Swedish sites.

Model simplification uncertainties in SR-Site

The modelling and its uncertainties are discussed in Sections 2.2.8 and 3.1.8.

Input data and data uncertainties in SR-Site

The input data and its uncertainties are discussed in Sections 2.2.8 and 3.1.8.

5.12.9 Adequacy of references supporting the handling in SR-Site

The theory of salt exclusion during permafrost conditions has been experimentally validated, supported by field observations, and published in the open literature. In common with the methane hydrate studies, there is limited evidence from crystalline rock occurrences in Fennoscandia and North America because of the complexity of climatic events. Most of the evidence is contained or referred to in the references cited.

5.13 Radiation effects (rock and grout)

5.13.1 Overview/general description

Radiation hazards from spent nuclear fuel derive from different types of radiation including α- and β-particles, neutrons and high-energy photons (γ and x-rays). Alpha- and beta-particles are effectively stopped by the first few millimetres of the waste package materials and x-rays also are rendered harmless by the same materials. Of greatest concern are the neutrons (plus associated secondary γ photons) and primary γ-radiation from each spent-fuel assembly. Both neutrons and γ-radiation are, in principle, able to penetrate through the waste package out into the buffer and adjacent rock.

Gamma radiation (from the spent fuel) that penetrates through the canister can decompose groundwater by radiolysis forming OH-radicals, hydrogen and oxygen molecules as well as several other species. Furthermore, gamma radiation can result in the breakdown of montmorillonite in the buffer material /SKB 2007, Allard and Calas 2009/. However, the net effect of the gamma radiation on the buffer material is considered to be unimportant because, a) the canister wall is sufficiently thick for the external effect of γ-radiolysis to be negligible, and b) any accumulated radiation dose in the buffer material will be insufficient to affect the montmorillonite. Therefore, gamma radiation effects are not expected to influence the buffer material or the near-field host bedrock.

Whereas γ-radiation is impeded by dense material through interactions with atomic electrons, neutrons are only slowed down by nuclear collisions, most efficiently with the light nuclei of hydrogen. Over periods of time, such sub-atomic disruptions can cause changes in the physical properties of the rock as well as of metallic and cementitious materials.

The major use of cement in repository construction is in the form of grouting to: a) reduce the groundwater inflow into the repository during construction and operation, and b) to provide rock support in the form of shotcrete to secure and protect the system of rock bolts and wire mesh /SKB 2004d/. For the former, the grout should have an acceptably low hydraulic conductivity (e.g. $< 10^{-12}$ $m \cdot s^{-1}$) and a physical and chemical compatibility with the host rock environment. It should be free from cracks and not undergo shrinkage or water and host rock interactions under open repository service conditions.

Neutron irradiation of concrete and cement can change their physical characteristics, for example, causing shrinkage, expansion and changes in physical properties. Some or all of these effects could be due to water radiolysis. It is worth pointing out that cement and grout are present only in limited quantities and generally at a substantial distance from canisters, and therefore these materials will be subject to very small neutron fluxes. Gamma radiation may also cause temperature increases resulting in hydration and hydrolysis and a general weakening of the cement, but as noted above, gamma radiation is likely to be of limited significance, if any, in the current context.

Although alpha radiation is the least penetrating of the three common types of radiation, it could affect existing fracture minerals after release from a penetrated canister in the event of extensive sorption of radionuclides and/or precipitation of secondary minerals of uranium in fractures. These radiation effects would be very local and the rock matrix would remain unaffected.

5.13.2 Dependencies between process and geosphere variables

Table 5-14 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.13.7.

Table 5-14. Direct dependencies between the process "Radiation effects (rock and grout)" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	No.	–	–	Yes. See text for details.	All	Process neglected; too low radiation fluxes.
Groundwater flow	No.	–	–	No.	–	–
Groundwater pressure	No.	–	–	No.	–	–
Gas phase flow	No.	–	–	Yes. Radiolysis may generate gas.	All	Process neglected; too low radiation fluxes.
Repository geometry	Yes. Will affect the spatial disposition of the radiation fluxes in relation to rock and grout.	All	Process neglected; too low radiation fluxes.	No.	–	–
Fracture geometry	No.	–	–	No.	–	–
Rock stresses	No.	–	–	No.	–	–
Matrix minerals	Yes. Rock composition would affect the decomposition products due to radiation.	All	Process neglected; too low radiation fluxes.	Yes. But the effect may be neglected.	All	Process neglected; too low radiation fluxes.
Fracture minerals	Yes. Fracture mineral composition would affect the decomposition products due to radiation.	All	Process neglected; too low radiation fluxes.	Yes. But the effect may be neglected.	All	Process neglected; too low radiation fluxes.
Groundwater composition	Yes. Groundwater composition would affect the products from radiolysis.	All	Process neglected; too low radiation fluxes.	Yes. But the effect may be neglected.	All	Process neglected; too low radiation fluxes.
Gas composition	No.	–	–	Yes. But the small amounts of gaseous radiolytic species are short lived and will not affect the composition of a gas phase.	All	Process neglected; too low radiation fluxes.
Structural and stray materials	Yes. Material composition would affect the decomposition products arising from neutron radiation.	All	Process neglected; too low radiation fluxes.	Yes. See text for details.	All	Process neglected; too low radiation fluxes.
Saturation	Yes. Water content affects radical production, lifetime and reactions. Radiolysis only takes place in water-saturated volumes.	All	Process neglected; too low radiation fluxes.	No.	–	–

5.13.3 Boundary conditions

The boundary condition is the radiation intensity to which the geosphere is exposed, i.e. the flux leaving the buffer/backfill surface.

5.13.4 Model studies/experimental studies

The Yucca Mountain Project /Tang 2000/ has carried out a series of calculations of radiation effects on ground support materials. The conclusion reached was that the cumulative fast neutron fluence at 295 years post emplacement is $2.11 \cdot 10^{13}$ n/cm2 which is significantly less than required to cause any structural damage. According to /Elleuch et al. 1972/, no degradation of the mechanical properties of cement have been observed for fast neutron fluence as high as $8.2 \cdot 10^{19}$ n/cm^2, i.e. no change in dimension, weight, compressive strength, bending strength, or Young's Modulus of cement paste due to irradiation alone.

The influence of gamma radiation on temperature increase was also addressed. The calculated incident gamma energy flux density at the drift wall following emplacement of the spent nuclear fuel was calculated to be $1.96 \cdot 10^8$ MeV/cm^2-s /CRWMS M&O 2000/. It is also known that for energy flux densities less than 10^{10} MeV/cm^2-s there is a negligible rise in temperature /ANSI/ANS 1997/. Since the temperature increase was negligible, it was concluded that the cement grout (and host bedrock) would be unaffected by gamma irradiation at the levels expected in a repository.

Furthermore, it must be pointed out that the Yucca Mountain repository concept does not include any buffer or backfill. Hence, larger radiation fluxes are to be expected in the rock mass for that concept as compared with the Swedish repository design. Yucca Mountain therefore represents a worst-case scenario, but still below the level of concern.

5.13.5 Natural analogues/observations in nature

Few observations of radiation damage on rock or cementitious materials have been reported from either observations in nature or studies of natural analogues. Some recent work, however, has reported the *in situ* radiation damage in diopside and calcite caused by α and recoil particles from nearby uranothorianite grains characterised by radiohaloes and radiating cracks resulting from swelling due to metamictisation /Seydoux-Guillaume et al. 2009/. The mineralogy and extent of the altered amorphous reaction zones in the calcite and diopside were quantified, showing good agreement between the measured thickness of the totally amorphous layer and that calculated using alpha and recoil nuclei ranges. Furthermore, /Utsunomiya et al. 2007/ using complex zoned zircons (partly amorphous) from granite examined the effects of radiation as a function of dose, in addition to the nano-scale microstructure and the composition of impurities and secondary alteration products. This showed that the concentrations of Ca and Al, which were considered to indicate alteration, increased dramatically at a cumulative dose of $1.6 \cdot 10^{16}$ (alpha-decay events/mg). In both cases, radiation effects give rise to alteration of rock-forming minerals and therefore a starting point for greater alteration.

5.13.6 Time perspective

This is determined by the decay properties of the spent fuel, see the SR-Site process report for fuel and canister /SKB 2010d/. The γ- and neutron-radiation fluxes leaving the canister are only significant for approximately the first 1,000 years.

5.13.7 Handling in the safety assessment SR-Site

Excavation/operation period and temperate climate domain

Calculations described above (Section 5.13.4) arrive at the overall conclusion that the neutron influence is too small to result in any detrimental changes in the mechanical properties of cement grout. In addition, any temperature increase from gamma irradiation (even at the maximum after spent fuel emplacement) is negligible. Therefore, the process is neglected.

Periglacial- and glacial climate domains

Lower radiation fluxes are expected during these periods. Therefore, the process is neglected also during these periods.

Earthquakes

Tectonic activity would have to be severe enough to cause breaching of the canister, mobilisation of radionuclides, and expose the host bedrock to increased radiation. The radiation effects on the integrity of the rock and fracture-filling minerals are not evaluated in SR-Site, but for such a scenario the retention or transport of radionuclides is not expected to be substantially affected by radiation effects, and therefore those effects are disregarded.

5.13.8 Uncertainties

There are no uncertainties of relevance to the safety assessment.

5.13.9 Adequacy of references supporting the handling in SR-Site

With respect to radiation effects on rock-forming minerals in the host rock, there is much published experimental work available, less so for *in situ* observations; these are reasonably covered above. In contrast, information on radiation effects on grouting materials is difficult to extract and there may be more information available.

The references /Allard and Calas 2009, Seydoux-Guillaume et al. 2009, Utsunomiya et al. 2007/ are peer-reviewed papers from the scientific literature. Other reports and publications that have not undergone a documented peer-review process /ANSI/ANS 1997, CRWMS M&O 2000, Elleuch et al. 1972, Tang 2000/ support the description of the radiation effects in the geosphere.

5.14 Earth currents

5.14.1 Overview/general description

Electric potentials and currents are present in soil as well as in rock. They originate from natural as well as anthropogenic sources /Enghag 2009a, b, Jones 1996, Kearey et al. 2002, Peabody 2001, Revie and Uhling 2008, Reynolds 1997, Sharma 1997, Sumner 1976/.

Currents caused by natural sources are called telluric currents or earth currents. They originate mostly from the interior of the earth, water currents in the ocean /Nolasco et al. 2006/, atmospheric discharges, the sun and the space in the universe /Enghag 2009a, b, Jones 1996, Kearey et al. 2002, Reynolds 1997, Sharma 1997, Sumner 1976/.

Anthropogenic currents are mostly referred to as stray currents although currents of natural origin might sometimes also be included. They originate mainly from transmission of electric power, rail transport, grounding to the (real) earth of various electric installations and radio communication /Jones 1996, Peabody 2001, Revie and Uhling 2008/.

In general, alternating electromagnetic fields become attenuated as they penetrate through soil and rock as a result of the skin effect (a tendency for the current density near the surface of a conductor to be greater than that at its core) /Kearey et al. 2002 (Figure 9.23), Reynolds 1997 (Figure 12.5), Sharma 1997 (Section 7.7.2)/. The lower the frequency and the higher the resistivity of the soil and rock in question, the deeper becomes the penetration. In concordance, electric fields are often strongest parallel to the ground surface and low perpendicular to it. Static electric fields which are high locally on the surface become weak at repository level for "geometrical" reasons[6].

The direct current (DC) components of naturally induced currents are small /Peabody 2001 (Chapter 11)/. The main origins are sea water currents /Nolasco et al. 2006/ (which give rise to

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[6] Strong and inhomogeneous local fields give rise only to weak and less varying fields at a distance.

electric potentials since they imply that charges move in the magnetic field of the Earth) and electrochemical effects in soil and rock /Mitchell 1993 (Section 12.18), Reynolds 1997 (Chapter 8)/ (in conjunction with electronic conductors such as pyrites and graphite/coal). The alternating current (AC) components of naturally induced currents are thus dominating. A considerable portion of these have low frequencies, such as periods of hours and days /Kearey et al. 2002 (Chapter 9), Reynolds 1997 (Chapter 10), Sumner 1976 (Chapter 6)/.

Most of the radiofrequency fields from anthropogenic sources are attenuated by the skin effect and do therefore not reach repository levels. Exceptions to this might include frequencies used in submarine navigation and radio communication. DC fields of interest in this regard include those from High Voltage Direct Current (HVDC) transmissions and certain rail transport systems. Electric grid frequency currents (50 Hz) may also reach repository levels.

Rectification effects are well known in the laboratory (e.g. the rectification cell comprising aluminium and copper electrodes in a salt solution) and in living organisms /Barnes and Greenebaum 2002/, but no mention of any natural non-biological rectifiers has been found in a limited information search.

External natural and anthropogenic fields that extend down to repository level may potentially influence the natural barriers by electrokinetic effects /Bard and Faulkner 2001 (Section 9.8), Mitchell 1993 (Section 12.18), Reynolds 1997 (Chapter 9), Sumner 1976 (Chapter 3)/. They are all expected to be weak, but electrophoresis and electroosmosis are assessed to be the least inefficient mechanisms /Bard and Faulkner 2001 (Section 9.8), Mitchell 1993 (Chapter 12)/. Electrochemical effects are not considered since there are no interfaces where the mode of conduction changes between ionic and electronic[7].

Electrophoresis takes place as a result of the forces acting on charged particles (ions) in an electric field. The forces are proportional to the charge of the ions in question. The motion is impeded by viscous effects which vary with size and other parameters. Consequently, different ions move with different velocities, even if the charge is the same. An external electric field might thus cause a separation of different ions.

Electroosmosis is another result of the forces acting on charged particles (ions) in an electric field. It takes place in systems having water in narrow pores. The surfaces of the pores are mostly negatively charged. Therefore, there is a surplus of positive charge in the "free" water. In an external electric field, the positive and negative ions drag the surrounding water in different directions. Since the positive charges are more abundant in the water, the net effect is that the water flows in the same direction as the positive charges.

Electrophoresis and electroosmosis are largely reversible, that is, the effect is eliminated if the direction of the external field is shifted to the opposite.

It is well known from corrosion of e.g. pipelines /Revie and Uhling 2008 (Section 12.1)/ that the effect of an alternating stray field may be a couple of orders of magnitude lower as compared with a direct current field having the same amplitude. The ratio is highly dependent on the mechanism of the interaction, however.

No mention has been found in the literature of any chemical changes in soil and rock appearing as a result of natural electric fields (with the obvious exception of atmospheric discharges). Effects of anthropogenic fields are typically found in connection with grounding of DC installations, in which case e.g. the pH of the porewater may change /Bard and Faulkner 2001, Jones 1996, Peabody 2001/. However, no changes are expected at repository level in crystalline rock as a result of any electrokinetic phenomena.

In conclusion, no effects of interest are expected to occur in the near field of a repository for spent nuclear fuel as a result of electrokinetic or electrochemical phenomena caused by natural and anthropogenic electromagnetic fields. The main reasons for this conclusion are given below.

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[7] Sulphides as well as some oxides in which the atoms have varying oxidation states may show electronic conductivity as well. Such minerals absorb visible light and are dark or show metallic luster. They do not form continuous paths of any significance in the types of rock considered for a Swedish repository for spent nuclear fuel, see page 4 in /Sumner 1996/.

- The fields are usually weak.
- Alternating fields are essentially eliminated by the skin effect.
- Most of the fields are alternating, in which case the effects are essentially reversible.
- There are no indications of any rectification effects.
- Local static electric fields at the surface are weak at repository levels for geometrical reasons.
- There are no interfaces where the mode of conduction changes between ionic and electronic.

5.14.2 Dependencies between process and geosphere variables

Table 5-15 show how electrokinetic processes are influenced by and influence all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 5.14.7.

Table 5-15. Direct dependencies between the process "Earth currents" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes.	All	Process neglected; too small electrical potential fields to affect groundwater flow or solute transport	No. But indirectly through the groundwater flow created by electro-osmosis. The effect is negligible. See row Groundwater flow.	–	–
Groundwater flow	No.	–	–	Yes.	All	Process neglected; too small electrical potential fields to affect groundwater flow or solute transport.
Groundwater pressure	No.	–	–	No. But indirectly through the groundwater flow created by electro-osmosis. The effect is negligible. See row Groundwater flow.	–	–
Gas phase flow	No.	–	–	No. But indirectly through the groundwater flow created by electro-osmosis. The effect is negligible. See row Groundwater flow.	–	–
Repository geometry	No.	–	–	No.	–	–
Fracture geometry	Yes. The processes take place in fractures. Their geometry will affect the direction of groundwater flow and solute transport.	All	Process neglected; too small electrical potential fields to affect groundwater flow or solute transport.	No.	–	–
Rock stresses	No. But indirectly through fracture geometry.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Matrix minerals	No.	–	–	No.	–	–
Fracture minerals	No. But indirectly through effects on groundwater composition.	–	–	No.	–	–
Groundwater composition	Yes. Electrophoresis acts on groundwater components.	All	Process neglected; too small electrical potential fields to affect groundwater flow or solute transport.	Yes. Electrophoresis affects the transport of groundwater components.	All	Process neglected; too small electrical potential fields to affect groundwater flow or solute transport.
Gas composition	No. But indirectly through effects on groundwater composition.	–	–	No. But indirectly through effects on groundwater composition.	–	–
Structural and stray materials	No. But indirectly through effects on groundwater composition.	–	–	No. But indirectly through effects on groundwater composition.	–	–
Saturation	Yes. Electro-kinetic processes may only occur in water-saturated rock.	All	Process neglected; too small electrical potential fields to affect groundwater flow or solute transport.	No.	–	–

5.14.3 Boundary conditions

The electric potential fields at the boundaries of the geosphere are the boundary conditions for electrokinetic processes.

5.14.4 Model studies/experimental studies

See "Overview/general description".

5.14.5 Time perspective

There are no special time aspects to these processes. They might occur whenever an electric potential field develops.

5.14.6 Natural analogues/observations in nature

See "Overview/general description".

5.14.7 Handling in the safety assessment SR-Site

Sufficiently large electric potential fields are not foreseen that may affect either groundwater flow or the transport of solutes in fractured granite by electrophoresis or electroosmosis. This applies to all periods and climatic conditions encountered during the assessment period of the repository. Therefore these processes are not considered in SR-Site.

5.14.8 Uncertainties

Uncertainties in mechanistic understanding

Electrophoresis and electroosmosis are well understood processes.

Model simplification uncertainties in SR-Site

Not relevant.

Input data and data uncertainties in SR-Site

Not relevant.

5.14.9 Adequacy of references supporting the handling in SR-Site

All references are books and the associated review process varies strongly with the type of book, subject area etc. The text in the books is supported by references with one exception, namely Peabody's book on corrosion. This is the second edition published in the year 2001. The first edition was published in 1967. According to the preface, "*every attempt has been made to check the accuracy of all the statements and other data*". The book was written originally by Peabody, but a number of authors have taken on in the second edition checking each others texts. The book is published by NACE International, The Corrosion Society of the United States.

All books have long acknowledgements showing that a number of persons have helped in each book to ensure a high quality.

Many books are popular books with the intent to spread scientific and technical knowledge to a wide audience with little knowledge in advance. None of the books cited belong to this category. Only the books by Per Enghag are written for a wider audience since they cover a wide area. Dr Enghag is an extremely qualified author who has previously produced the "*Encyclopedia of the elements*" published by Wiley-VCH. The books about the Earth have the same quality, but they have not yet been translated into English.

6 Radionuclide transport processes

6.1 Transport of radionuclides in the water phase

6.1.1 Overview/general description

A number of processes will, or could, influence the transport of radionuclides in the water phase: advection and dispersion (mixing), diffusion and rock-matrix diffusion, sorption and speciation, colloid transport and radioactive decay. All these processes have been discussed above among the processes occurring in the geosphere, or, in the case of decay, under fuel processes (see SR-Site process report for fuel and canister /SKB 2010d/).

In this section, the integrated aspects of these processes and their handling in the safety assessment SR-Site are discussed. The main transport processes of radionuclides and the modelling of these processes have been the focus of the EU-project /RETROCK 2004, 2005/ involving both implementers, including SKB, and a regulator. The approach adopted in SR-Site and described below is heavily based on the RETROCK conclusions and experiences from SR-Can. The general description in the following paragraphs is also taken, in shortened form and modified according to SR-Site as needed, directly from /RETROCK 2005/.

The dominating transport mechanism for solutes in fractured rock is with the flowing groundwater. Since water flow is restricted to the fractures, the dimensions, shape, orientation and connectivity of the fractures determine the properties of the flow paths in the rock. Very small-scale features of the fractures, such as aperture variations, may have an important influence on the flow paths. Preferential flow paths or channels may develop through parts of the fractures with larger aperture. Of special interest are fast flow channels with a very small interaction area with the rock.

The migration rate of a radionuclide is usually much lower than the velocity of water. This is due to two general retention mechanisms: first, radionuclides in the fracture network enter the internal porous network of the rock matrix by diffusion, and second, radionuclides are removed from the aqueous phase by adsorption, surface precipitation and co-precipitation, and deposited onto the mineral surfaces of the rock or fracture fillings.

The coupling between retention and flow characteristics is usually referred to as flow-related transport resistance or hydrodynamic control of retention, and is in SKB applications denoted by F [T/L]. The important quantity is the ratio between the mass flux into the matrix and the mass flux in the flowing water. In the simplified case of a uniform fracture of width W and length L, this ratio is proportional to the area of the fracture ($2WL$ or "flow wetted surface area") divided by the groundwater flow rate Q in the fracture. For a fracture network, a summation is made over all fractures i along a flow path; i.e. the flow-related transport resistance is given by $F = 2\sum_i W_i L_i / Q_i$. In the general case of heterogeneous and intersecting fractures, it can still be shown that the important entity WL/Q for the flow paths always can be determined once the flow and the geometry of the flow field is known. In this case, the transport resistance is defined as $F = \int dl/(v(l)b(l))$ where integration is performed along the pathline and v and b are the particle (solute) velocity and fracture half-aperture, respectively. It is noted that both these entities are functions of the distance along the pathline. The flow-related transport resistance is defined in e.g. /Cvetkovic et al. 1999/ and also used in e.g. /Painter et al. 2008/; however, in these references this entity is denoted by β. Within SKB modelling applications, a comprehensive discussion on the flow-related transport resistance is provided in /Crawford and Sidborn 2009/.

Matrix diffusion is caused by random movement, which, in the presence of concentration gradients, causes a net movement of solute. In SR-Site it is assumed that the pore space of the matrix is connected over all distances of interest within the assessment /SKB 2010b, Section 6.8/. Thus, it is the fracture spacing (strictly half-spacing) that governs the penetration depth. Depths of a few centimetres are sufficient to make matrix diffusion an effective retarding process. After entering the pore system, the solutes may sorb on the extensive pore surfaces. For non-sorbing species, it is also important that matrix diffusion extends the residence time, increasing the time for radioactive decay. Since the mineral surfaces are most often negatively charged under natural conditions, there is a repulsion of negatively charged ions close to the surfaces, which can decrease matrix diffusion. Another potentially decreasing effect could be pore clogging caused by the precipitation of e.g. cementitious compounds from the engineered barriers. An analogous effect in fractures, fracture clogging, would reduce the water flow and thus increase the travel times. It is noted that sorption includes several different mechanisms, e.g. ion-exchange, physical adsorption and surface complexation. These processes are discussed in more detail in Section 5.4.

The radionuclides can be dissolved in groundwater in ionic form, as constituents of chemical compounds, or attached to various waterborne particles like colloids or microbes. The number of chemical factors affecting concentrations of radionuclides in groundwaters is large. Mineralogy, aqueous speciation and the solubility of derived phases are likely to constitute the major controls. The potential of geologic formations to provide reactants is vast, but the groundwater brings reactants also from the repository near field and from the ground surface. The conditions deep in the bedrock are normally strongly reducing, which promotes the retention of some redox-sensitive radioelements.

If a radionuclide is present at concentrations exceeding the solubility of a solid phase, it precipitates from solution. The solubility depends strongly on the existence of complexing agents and solubility-limiting solid phases. The concentrations of the radionuclides in the far-field groundwaters are negligible from the chemical viewpoint. This is true also for uranium despite its significant amount in the waste. The large reducing capacity of iron oxides, such as magnetite, and the low oxidative capacity of the groundwater for the hydrogeochemical conditions expected at the site, results in only a very small release of uranium into the far field. As a consequence, the influence of radionuclides on other substances in the geosphere is negligible. In some cases, it should be taken into account that a radioelement can migrate together with much more abundant inactive isotopes of the same element (i.e. ^{90}Sr with ^{88}Sr). It is possible that radionuclides first precipitate and later, following a change in groundwater chemistry, become rapidly dissolved. However, owing to the geochemical stability (through buffering capacity of the geosphere), the potential for such transient situations becomes smaller with increasing depth.

The attachment of radionuclides to minute particles, or colloids, in groundwater involves a large variety of possible developments. Site investigations have revealed typically low concentrations of colloids and other particles suspended in groundwater, which suggests a low relevance to migration of radionuclides in natural groundwaters. The attachment can be reversible or irreversible, and the particles can be mobile or immobile. Furthermore, the size and composition of particles can change with time, and microbes add complexity to the system with their metabolic processes. The largest particles are mechanically filtered within a fracture, whereas the smallest ones are transported with the water flow, carrying radioelements possibly faster than they would move alone.

6.1.2 Dependencies between process and geosphere variables

Table 6-1 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Site is also indicated in the table and further described in Section 6.1.7.

Table 6-1. Direct dependencies between the process "Transport of radionuclides in water phase" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	Yes. Since temperature affects the type and extent of the chemical and physical retardation processes, and also indirectly through viscosity and density, which affects flow.	Excavation/operation	Process not relevant.	No.	–	–
		Temperate	Sorption coefficients and matrix diffusivities are chosen for relevant temperature conditions.			
		Periglacial	See Temperate above.			
		Glacial	See Temperate above.			

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Groundwater flow	Yes. Groundwater flow governs transport.	Excavation/ operation/	Process not relevant.	No.	–	–
		Temperate	Flow paths, Darcy flux, flow-related transport resistance, advective travel time from site-specific groundwater flow modelling, see Section 3.1			
		Periglacial	See Temperate above.			
		Glacial	See Temperate above.			
Groundwater pressure	No. But indirectly since pressure affects flow.	–	–	No.	–	–
Gas phase flow	No. But indirectly, since gas flow affects groundwater flow.	–	–	No. Does not affect gas flow.	–	–
Repository geometry	Yes. Repository geometry affects distribution and characteristics of flow paths, and hence transport, to the surface.	Excavation/ operation	Process not relevant.	No.	–	–
		Temperate	Flow paths and characteristics from site-specific groundwater flow modelling where tunnel layout is implemented in the models, see Section 3.1.			
		Periglacial	See Temperate above. However, repository not explicitly included in groundwater flow model incorporating permafrost.			
		Glacial	See Temperate above. However, repository not explicitly included in groundwater flow model incorporating an ice sheet.			
Fracture geometry	Yes. Fracture network geometry governs flow and hence non-reactive transport characteristics.	Excavation/ operation	Process not relevant.	No. Amounts of transported radionuclides are negligible in terms of mass.	–	–
		Temperate Periglacial Glacial	Flow-related transport resistance from site-specific groundwater flow modelling, see Section 3.1. Site-specific porosities and formation factors considered in the selection of matrix porosity and diffusivity, see Section 5.3. Site-specific porosities, BET surfaces and stress effects considered in the selection of Kd values, see Section 5.4.			
Rock stresses	No. But indirectly since stress affects fracture aperture and flow.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Matrix minerals	Yes. For diffusing species, matrix minerals affect sorption behaviour in matrix and also the extent of diffusion.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Site-specific rock mineralogy considered in the selection of sorption data, see Section 5.4.	No. If reactions occur, mineral changes could occur, but these are considered to be of negligible significance.	–	–
Fracture minerals	Yes. Fracture minerals affect fracture surface sorption and also access to matrix through diffusion.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Site-specific fracture mineralogy considered in the selection of sorption data, see Section 5.4. However, surface sorption not invoked in SR-Site.	No. If reactions occur, mineral changes could occur, but considered second order effect.	–	–
Groundwater composition	Yes. Composition affects speciation of radionuclides, and hence their transport characteristics.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Site-specific water salinity, pH, redox, organic acids, microbes considered in the selection of sorption and diffusion data, see Sections 5.3 and 5.4.	Yes. Transport of dissolved species affects the water composition, but radionuclide transport is not of importance to understand major chemistry.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Radionuclide concentration and release to the biosphere are calculated.
Gas composition	No. But indirectly through dissolution in groundwater some gases (e.g. O_2, CO_2 and H_2) affect radioelement speciation.	–	–	No. But indirectly through effects on groundwater composition.	–	–
Structural and stray materials	Yes. Sorption on stray materials affects transport characteristics, but this is primarily a near-field rather than a far-field issue.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Sorption on structural and stray materials in the geosphere neglected.	No.	–	–
Saturation	No. But indirectly, since saturation affects groundwater flow.	–	–	No.	–	–

6.1.3 Boundary conditions

The inner boundary condition is the concentration of radionuclides in the water phase leaving the engineered barriers. The radionuclide flux from the engineered barriers (buffer and backfill) constitutes the input for the transport in the geosphere. For model application in SR-Site, see below.

The outer boundary is the geosphere-biosphere interface zone, or alternatively, the vertical and/or bottom boundary of the groundwater flow simulation domain.

6.1.4 Model studies/experimental studies

Experimental studies of individual processes are discussed above; experimental studies of the combined processes under spatial and temporal scales corresponding to the scales of relevance for performance assessment applications do not exist. However, for shorter scales, the TRUE-1 /Winberg et al. 2000, Widestrand et al. 2007, Cvetkovic et al. 2007, Cvetkovic and Cheng 2008/ and

TRUE Block scale /Poteri et al. 2002, Winberg et al. 2003, Neretnieks and Moreno 2003, Cvetkovic et al. 2010, Cvetkovic and Frampton 2010/ experiments have shed light on the predictive capability using models based on the same processes as described above. In short, the TRUE experience indicates an adequate understanding of the relevant processes.

Model studies for spatial and temporal scales of relevance for safety assessment applications have been performed in earlier performance assessment studies (e.g. SR 97 and SR-Can), but most notably in the recently finalised Task 6 of the Äspö Task Force on modelling of groundwater flow and transport of solutes /Hodgkinson and Black 2005, Hodgkinson et al. 2009, Gustafson et al. 2009, Moreno and Crawford 2009/. There, a comparison has been made between models with a detailed description of processes and more traditional safety assessment models where a higher level of process abstraction is made. Specifically it has been studied how these models scale in time and space when going from typical experimental time and space scales to safety assessment scales. Also, these studies confirm that the processes discussed above are adequate for application to the scales of interest for performance assessment. However, the type of processes that typically dominate tracer experiments (e.g. sorption on fracture surfaces and diffusion into fracture rim zones with subsequent sorption) are not necessarily of interest on the longer timescales.

6.1.5 Natural analogues/observations in nature

Supporting evidence from natural analogues and observations in nature are discussed in conjunction with the individual processes described in Chapter 5. Natural analogue evidence is not directly applicable for the integrated transport model, but some aspects of transport can be studied in such analogues. For example, a natural analogue for matrix diffusion of a transported solute has been found in connection with an oxidation front of uranium mineralisation in Poços de Caldas /MacKenzie et al. 1992, Romero et al. 1992/. Infiltrating oxygen-rich water from the surface has there caused oxidation along a fracture and in the unfractured rock matrix adjacent to the fracture.

Other analogues studies are summarised in /Miller et al. 1994, 2000/.

6.1.6 Time perspective

All timescales after canister failure are relevant for transport of radionuclides in the water phase.

6.1.7 Handling in the safety assessment SR-Site

Excavation/operation period

The process is of no relevance for this period, since the engineered barriers are considered to be intact.

Temperate climate domain

The most detailed analysis of radionuclide transport is performed for the initial temperate climate domain. The modelling of this period, which is partially exemplified in the SR-Can report /SKB 2006b/, is based on the code FARF31/Norman and Kjellbert 1990/ and MARFA /Painter and Mancillas 2009/. The transport along path lines from individual canisters to the biosphere is described. The flow paths are obtained from groundwater flow modelling, cf. Section 3.1. The results that are transferred from the flow models to FARF31 and MARFA are the flow-related transport resistance and advective travel time from the canister deposition locations to the biosphere. Thus, flow modelling and transport modelling are decoupled.

FARF31 solves the transport equations along the one-dimensional path lines (conceptualised as streamtubes) based on a dual porosity description with advection-dispersion in the mobile phase (flowing water) and diffusion into the immobile water in the rock matrix. An exchange term between the two phases is included in the governing equations. A finite penetration depth for radionuclides is assumed in the model (based on fracture half-spacing). In the matrix, the radionuclides are subject to sorption described using the linear equilibrium K_d concept. The main simplification made is that only steady-state flow-fields can be handled. In practice, this means that particle tracking results for a snapshot in time (implying stationary flow for the selected snapshot) from the transient groundwater flow models are used, cf. Section 3.1.

MARFA (Migration Analysis of Radionuclides in the Far Field) uses a particle-based Monte Carlo method to simulate the transport of radionuclides in a sparsely fractured geological medium. The physical processes represented in MARFA include advection, longitudinal dispersion, Fickian diffusion into an infinite or finite rock matrix, equilibrium sorption, radioactive decay and in-growth. Multiple, non-branching decay chains of arbitrary length can be handled. MARFA uses the particle on random streamline segment algorithm /Painter et al. 2006/, a Monte Carlo algorithm combining time-domain random walk methods with stochastic pathway simulations. The algorithm uses non-interacting particles to represent packets of radionuclide mass. These particles are moved through the system according to rules that mimic the underlying physical transport and retention processes. Because the algorithm uses non-interacting particles, the transport and retention processes are limited to those that depend linearly on radionuclide concentration. Nonlinear processes such as solubility-limited transport or aqueous speciation cannot be represented. MARFA is specifically designed to work with output from discrete fracture network (DFN), continuous porous medium (CPM), or nested DFN/CPM flow models. A scientific paper high-lighting the methodology MARFA is based on and providing illustrative computational examples has been published in /Painter et al. 2008/.

The main advantage of MARFA relative to FARF31 is that different retention models can be specified for different sub-units of the system, e.g. different models for hydraulic rock, hydraulic conductor (deformation zone), and hydraulic soil domains. Furthermore, also the engineered part of the system, i.e. tunnels, can be assigned retention. Finally, the flow magnitude, but not direction, can be changed along the pathlines. This provides an opportunity to address, in at least an approximate sense, e.g. glacial conditions where flow may be almost stagnant during ice-sheet coverage, but very high when the ice-sheet margin passes above the repository. In a future version being developed during the SR-Site project, fully transient flow conditions will be accommodated. However, application results will be available only after completion of SR-Site.

Colloid-facilitated transport (CFT), which is not included in FARF31, can be handled using a finite volume version of FARF31 denoted FARF33 /Vahlund and Hermansson 2006/. In FARF33, the governing equations are discretised using a finite volume scheme, and solved numerically using an iterative solver. Also more complicated boundary conditions and matrix heterogeneity can be handled. However, in SR-Site CFT is handled using two alternative approaches; the colloidal material is assumed to be bentonite particles from the backfill rather than naturally occurring colloids. For rapid reversible sorption/desorption onto colloids, an expression that modifies the MARFA input parameters which quantify radionuclide retention in the host rock matrix is derived. Irreversible sorption onto bentonite colloids is handled by considering one mitigating process only; i.e. a finite number of sorption sites are available on the colloids. The radionuclides must thus compete for these available sites. For all other processes and parameters, pessimistic or bounding approximations are used. These include; no desorption from colloids, the forward sorption rate is infinitely fast, no colloid retardation or filtration, colloids do not enter rock the matrix, colloid concentration is constant along each pathway, and colloid concentration is constant in time. Based on these approximations, the distribution of radionuclides between dissolved and colloid-associated radionuclides can be determined in the near-field transport code COMP23. This input is then used directly in radionuclide transport calculations in MARFA. It is noted that irreversible sorption is not included in the compliance calculations in SR-Site based on arguments provided in the buffer, backfill and closure process report /SKB 2010e/.

Separate FARF31 and MARFA models are set up for the cases involving transport starting i) from a fracture intersecting the deposition hole (Q1 path), ii) from the EDZ (Q2 path), and iii) directly from the tunnel and into a fracture intersecting the tunnel (Q3 path). The three paths Q1, Q2 and Q3 correspond to the conceptualisation of transport in the near field as implemented in the code COMP23. In FARF31, the transport times in the EDZ and the tunnel are neglected; i.e. for all three paths, only the travel time in the rock is accounted for. In MARFA, transport and retention in tunnels is analysed in detail.

The main inputs to the above analyses are the groundwater flow simulations for the Temperate period (cf. Section 3.1), and radionuclide transport characteristics based on the site-descriptive model and the data compilation undertaken within the SR-Site assessment /SKB 2010b/. Also, the tunnel layout is needed for assigning starting positions for particles in the groundwater flow model.

Periglacial climate domain

The simulation of groundwater flow during periglacial conditions aims at establishing groundwater flow patterns during the period when the site is subject to permafrost but no ice sheet is present. A large super-regional domain needs to be considered for these simulations.

Radionuclide transport during the periglacial climate domain is handled in a simplified manner. The pathlines obtained in the groundwater flow simulations for temperate conditions are used, but advective travel time and flow-related transport resistance are scaled based on the flow ratio between the periglacial- and temperate flow simulations. In addition, K_d-values and colloid concentrations are chosen to reflect the groundwater chemical conditions of the periglacial climate domain.

Glacial climate domain

The simulation of groundwater flow during a glacial advance and retreat aims at establishing groundwater flow patterns during the period when an ice sheet builds up, passes and retreats over the repository. Permafrost may or may not be present depending on assumptions made. A large super-regional domain needs to be considered for these simulations.

Radionuclide transport during the glacial period is handled in a simplified manner. The pathlines obtained in the groundwater flow simulations for temperate conditions are used, but advective travel time and flow-related transport resistance are scaled based on the flow ratio between the glacial and temperate flow simulations. In addition, K_d-values and colloid concentrations are chosen to reflect the groundwater chemical conditions of the glacial climate domain. Several different sub-regimes within the glacial period may be identified.

The evolution over a full glacial cycle using these scaling factors is modelled in MARFA where temporal changes in velocity and retention properties can be accommodated.

Earthquakes

The potential impact of earthquakes is illustrated by simple calculations where no credit is taken for radionuclide transport and retention in the geosphere. This is motivated by the fact that shear displacement is expected to occur in larger fractures, where the transport resistance is initially low. Furthermore, the retention characteristics of these fractures after the shear displacement event are essentially unknown.

6.1.8 Uncertainties

Uncertainties in mechanistic understanding

Uncertainties in the individual processes are discussed in the relevant sections describing each process; model implementation and data issues are covered in the following subsections.

Model simplification uncertainties in SR-Site

The conceptualisation of velocity variations as a dispersion process and its implementation in FARF31 results in some uncertainty. Dispersion/mixing along the individual flow paths is, in FARF31, modelled by means of a dispersion term, which is expressed through the dimensionless Peclet number that quantifies the ratio between advective and dispersive transport. The effect of the chosen value on results is small; hence also the effect of the associated uncertainty on results is small. However, it is noted that the approach in FARF31 using the flow path integrated flow-related transport resistance value is based on an assumption of no dispersion. Hence, inclusion of dispersion in the calculations adds to the uncertainty in the sense that an underlying assumption is not fully met.

In MARFA, a longitudinal dispersivity is assigned; however, this can be set to zero. It is also noted that in MARFA, no assumption of zero dispersion is needed in order for the solution to be formally correct.

Concerning the matrix diffusion term, the largest uncertainty is related to how the transport resistance is calculated. The concept is easily interpreted in a geometrically simplified model of fracture flow, but the question is whether such models can realistically describe the effect of matrix diffusion under natural flow conditions where channelling occurs. In the discrete fracture network models for groundwater flow, cf. Section 3.1, aperture heterogeneity is typically not included. Also, when flow paths are extracted from continuum models where individual fractures are not described, (constant) values for the flow-wetted surface per unit volume of rock are needed. These values are highly uncertain even if they can be related to fracture statistics such as e.g. P_{32} values or conductive fracture frequency. In SR-Site, it is argued in the radionuclide transport report /SKB 2010n/ that no reduction in flow-related transport resistance due to channelling should be applied. This is based on calculations showing that if channelling occurs, there is also diffusion into stagnant water zones next to the channels in the fracture plane. The diffusion into these stagnant water zones is accompanied by subsequent diffusion into the matrix. The formation of stagnant water thus compensates the effects caused by channelling.

Concerning sorption, the uncertainties are more of a mechanistic nature than related to modelling. Specifically, the simplification of adopting the K_d-approach implies uncertainties as discussed in Section 5.4. Furthermore, the process of sorption on colloidal material is associated with relatively large uncertainties. These uncertainties concern whether the process is reversible or not, and the actual concentrations of colloidal material that are present in the groundwater. The process is of limited relevance for the overall safety of the repository when naturally occurring colloids are considered, since high concentrations of colloidal material rarely occur naturally in the site-specific groundwaters of interest. However, bentonite colloids resulting from erosion, especially during conditions with dilute glacial meltwaters potentially reaching repository depth, may imply large consequences on the overall safety. Here the uncertainties are more problematic, and pessimistic assumptions are necessary in the assessment within SR-Site.

In /RETROCK 2005/ it was discussed at some length if the coupling of the individual processes, as embodied though the governing equations implemented as e.g. in FARF31, implies an additional integrated model uncertainty relative to the uncertainty of the individual processes. No such uncertainty was identified.

Input data and data uncertainties in SR-Site

Input data for the radionuclide transport calculations come from two sources: i) flow-related transport parameters (F and t_w) from the groundwater flow simulations, and ii) radionuclide sorption and diffusion data from the SR-Site Data report /SKB 2010b/. The sorption data, which are based on the site-descriptive models and a general assessment of existing data and associated uncertainties, are also presented in a supporting document /Crawford 2010/. Concerning diffusion data, several supporting documents are used, see further the SR-Site Data report /SKB 2010b/. The diffusion data compilation also includes values for matrix penetration depth and matrix porosity. An overall assessment of the associated uncertainties affecting modelling is made in the SR-Site Data report /SKB 2010b/. The main uncertainties in sorption data are related to different laboratory techniques being subject to different measurement uncertainties. These are primarily associated with effects of additional surfaces if crushed samples are used, or stress and decompression effects if whole samples are used.

Additionally, parameter values are needed for radionuclide half-lives and Peclet numbers. The radionuclide half-lives are generally known with great certainty (except for ^{79}Se), and the Peclet number is varied as described above.

6.1.9 Adequacy of references supporting the handling in SR-Site

The supporting references in this section are mainly peer-reviewed scientific papers. This is particularly true for the papers summarising the model and experimental studies the suggested methodology is based on. The main SKB reports cited are reports describing the numerical codes. Concerning FARF31, it is noted that a model validity report /Elert et al. 2004/ has been produced, while the methods implemented in MARFA are scientifically published in /Painter et al. 2008/. The concepts concerning the flow-related transport resistance are discussed in /Cvetkovic et al. 1999, Painter et al. 2008, and Crawford and Sidborn 2009/.

Older SKB reports have undergone documented factual and quality reviews, but these are not necessarily documented according to SR-Site standards.

6.2 Transport of radionuclides in the gas phase

6.2.1 Overview/general description

The flow of gas in the geosphere is described in Section 3.2. This section describes how radionuclides can be transported by a gas phase.

At the pore-fluid pressure prevailing in a deep repository, some radionuclides or compounds containing radionuclides that would exist in gaseous form at atmospheric pressure will be dissolved in the aqueous phase. These radionuclides are then transported as solutes, whose transport has been described in Section 6.1.

If a free-gas phase is present, radionuclides that are themselves gaseous or that are present in volatile or gaseous compounds can partition into the gas phase and be transported with the gas. As indicated in Section 3.2.1, the natural concentrations of dissolved gases are not expected to be sufficient in themselves to form a gas phase at the water pressure prevailing at repository depth. A scenario in which a free gas phase might form is where the corrosion of a defective canister generates bubbles of free gas. Only radionuclides that can exist in the gas phase, either in their own right (e.g. noble gas isotopes) or as part of a gaseous compound (e.g. $^3H^1H$) can be transported directly with the migrating free gas. This applies only to a few radionuclides. The concentrations of these radionuclides in the gas are controlled by the partial pressures, solubilities, and rates of generation of the gaseous species containing the radionuclides.

Colloidal particles can also be transported with gas bubbles /Wan and Wilson 1994a/. The concentration of colloids in deep groundwaters is low and of no importance in this context, but experiments show that colloidal particles arising from bentonite buffer material can also attach to gas bubbles /Wan and Wilson 1994b/. If this is correct, it means that bentonite particles, including contaminated bentonite particles, could accompany gas bubbles. There is thus a possibility of indirect transport of radionuclides with gas bubbles from a damaged canister.

The possibility that migrating gas may modify groundwater flow velocities in the neighbourhood of the migrating gas and thereby influence transport of radionuclides dissolved in groundwater is discussed in Section 6.1.

6.2.2 Dependencies between process and geosphere variables

Table 6-2 shows how the transport of radionuclides in the gas phase is influenced by and influences geosphere variables and other geosphere processes. The handling in SR-Site is also indicated in the table and further described in Section 6.2.7. It is assumed that radionuclides that might be present in the gas phase are only present in trace quantities that would not affect the gas-phase properties.

Table 6-2. Direct dependencies between the process "Transport of radionuclides in the gas phase" and the defined geosphere variables and a short note on the handling in SR-Site.

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Temperature in bedrock	No. But indirectly through gas flow and gas composition since temperature affects viscosity, density, and gas solubility.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Groundwater flow	No. But indirectly through gas flow since groundwater flow affects gas flow and through changes in water composition since dissolved gases may come out of solution.	–	–	No.	–	–
Groundwater pressure	No. But indirectly since pressure affects groundwater flow, and hence transport as above.	–	–	No.	–	–
Gas phase flow	Yes. Gas flow governs transport in gas phase.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	No.	–	–
Repository geometry	Yes. Could influence radionuclides in gas phase leaving the near field.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	No.	–	–
Fracture geometry	Yes. Fracture network governs flow and hence transport.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	No. But indirectly since deposition of transported material could in principle block minor flow paths, but no volatile radioactive species have been identified that could do this to a significant degree.	–	–
Rock stresses	No. But indirectly since stress affects fracture aperture and flow.	–	–	No.	–	–
Matrix minerals	Yes. For diffusing species, matrix minerals affect sorption behaviour in matrix.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	No. If reactions occur, mineral changes could occur, but considered second order effect.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)	Influence present? (Yes/No? Description)	Time period/ Climate domain	Handling of influence (How/If not – Why)
Fracture minerals	Yes. Fracture minerals affect fracture surface sorption and also access to matrix through diffusion.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	No. If reactions occur, mineral changes could occur, but considered second order effect.	–	–
Groundwater composition	Yes. Groundwater composition affects gas composition, and hence transport in gas phase.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	Yes. Solutes transported in gas phase may later dissolve, and hence affect groundwater composition.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered, since all gas is assumed to be released to the biosphere.
Gas composition	Yes. Gas composition could affect chemical state of gaseous radionuclides and hence partitioning between phases, but no significant example identified.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	Yes. Transport of gaseous radionuclides can modify gas composition but only by trace amounts.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.
Structural and stray materials	Yes. But, gaseous radionuclides not expected to sorb significantly to these materials.	Excavation/ operation Temperate Periglacial Glacial	Process not relevant. Not considered since geosphere is short circuited and release of radionuclides in gas phase is assumed to occur from the near field to the biosphere.	No.	–	–
Saturation	No. But indirectly, since saturation affects gas phase flow, and hence transport in gas phase.	–	–	No.	–	–

6.2.3 Boundary conditions

The magnitude and characteristics of the gas-phase flow are the principal controlling factors in the transport of radionuclides in the gas phase.

The additional boundary conditions required are those to determine the concentrations of the radionuclides in the gas phase. This may include the concentration in the gas stream leaving the near field. It could also include the concentrations of the radionuclides in groundwater in contact with the gas stream; these radionuclides may partition into the gas stream.

The outer boundary is provided by the geosphere-biosphere interface zone (it is assumed that the gas flow will be predominantly vertical, unless forced to migrate laterally by some horizontal low permeability or capillary barrier). If, as expected, the flow is advection dominated, the variation of conditions at the surface, within the range that is credible, will not have a significant effect on transport of radionuclides by gases to the surface.

For the case of sorption of radionuclides onto particles attached to the surface of gas bubbles, the degree of sorption will depend on the concentrations in the groundwater through which the bubbles pass.

6.2.4 Model studies/experimental studies

Transport of components of a gas phase through porous materials is a well understood process, both experimentally and theoretically. Whether the components are radioactive or not is immaterial to this understanding. Given the knowledge of the flow of a gas phase through the geosphere, the assessment of radionuclide transport in the gas phase is considered relatively straightforward. There is some difficulty in assessing the extent to which components in the gas phase may partition into the water phase, arising mainly from the difficulty in determining how much groundwater the migrating gas comes into contact with. Characterising the gas-phase flow itself is, however, the main assessment difficulty, as discussed in Section 3.2.

A modelling study has been carried out to ascertain the importance of transport of radionuclides attached to gas bubbles /Neretnieks and Ernstson 1997/. In that study, it was assumed that all gas from a damaged canister is released in the form of small bubbles covered with montmorillonite particles from the bentonite buffer. The clay was further assumed to have sorbed radionuclides from the leaching of the fuel. The particles were assumed to remain irreversibly bound to the bubbles, while all gas was assumed to reach the ground surface. The actinides remained irreversibly bound to the clay particles, whereas caesium and strontium desorbed from the bentonite clay and underwent matrix diffusion combined with sorption during transport through the rock. The results of the calculations showed that the releases to the biosphere were very limited for all radionuclides even with these pessimistic assumptions.

The migration of a free gas through an otherwise water-saturated sparse fracture network will take place along channels controlled by the geometry of the connected fracture network and the spatial variability of fracture apertures. Gas-phase flow paths are often subject to instabilities, with a free gas pathway collapsing and reforming, resulting in the formation of separated bubbles, known as Hele-Shaw bubbles. Characteristics of gas transport through single water-saturated fractures have examined in a number of laboratory experiments and modelling studies (see, for example, /Hoch et al. 2001/ and /Rodwell et al. 1999/). The capacity for gas migration through the fractured rock at Forsmark was considered as part of the SR-Can Assessment /Hartley et al. 2006a/.

6.2.5 Natural analogues/observations in nature

Attempts have been made to identify transport of substances through the geosphere as gases or attached to gas bubbles. Undoubtedly, near the surface, gas-phase transport occurs from below the water table in some areas (leaving aside volcanic systems), but there can be difficulty in determining whether gas-phase transport started at depth or whether gases were transported in solution at depth and only formed a separate gas phase closer to the surface. A review of "geogas" migration can be found in /Goodfield and Rodwell 1998/ and the references therein, and discussion can also be found in /Rodwell 2000/. Natural analogue studies have not yet contributed significantly to the validation of assessments of gas migration from a repository.

6.2.6 Time perspective

All timescales after canister failure, while radionuclides that could be transported by migrating gas are still being released, are of interest as gas generation could continue for a long while into the future. The timescale for the transport of gas bubbles and components of a gas phase through the geosphere can be much faster than advective water transport.

6.2.7 Handling in the safety assessment SR-Site

Excavation/operation period

No transport of radionuclides is expected for this period, and it is thus excluded from the assessment. It will be long after repository closure before the buffer becomes resaturated and there is the possibility for any groundwater to enter a defective canister and initiate hydrogen gas production from corrosion of the iron insert.

Temperate-, periglacial- and glacial climate domains

In the safety assessment, transport in the gas phase is treated pessimistically as a short circuit of the repository to the biosphere, i.e. transport through the geosphere is neglected. As long as this cautious approach shows that transport of gaseous radionuclides cause no significant hazard, it is not necessary to examine the details of the migration process. The gaseous radionuclides assessed in this way are ^{14}C, presumed to be present as methane or carbon dioxide, and ^{222}Rn.

Transport via colloidal material that is transported with gas bubbles is not taken into account in the safety assessment. This is justified by the model studies described above.

Earthquakes

The potential impact of earthquakes is neglected since transport in the gas phase is already treated as a short circuit of the repository with the biosphere.

6.2.8 Uncertainties

Uncertainties in mechanistic understanding

The process for transport of gaseous radionuclides in a gas phase or in gas bubbles is well understood. By contrast, sorption of colloids on gas bubbles is associated with considerable uncertainties. However, this process is of minor importance for overall safety.

Model simplification uncertainties in SR-Site

The consequences of the transport of radionuclides by migrating gas are assessed using a model that neglects the transport through the geosphere – the geosphere is effectively short circuited, with gas generated at the repository being approximated as moving directly into the biosphere. This is a gross simplification of the transport process, but is a robust treatment for evaluation of the consequences. The main approximation made in this approach is neglecting the fraction of the generated gas that dissolves in the groundwater and may then have a significant travel time. Neglecting the travel time of the free gas is expected to be a minor approximation, because the travel time will be short. However, for short lived nuclides such as e.g. ^{222}Rn, the assumption of a zero travel time in the gas phase may be pessimistic since decay could be important.

Input data and data uncertainties in SR-Site

Uncertainties in the assessment of the transport of radionuclides as a component of a migrating gas derive from uncertainties in the characteristics of gas flow to the surface (i.e. the details of the flow paths that the gas would follow are not well established and the extent to which the flow will occur via stable gas-filled pathways, through changing, unstable pathways, or as bubbles is uncertain) and on the quantification of release of radionuclides in gaseous form. However, since cautious assumptions about the release of gaseous radionuclides and an assumption of instantaneous transport to the surface show insignificant hazards from this release pathway, the uncertainties are of no consequence.

Assessment of the transport of sorbed radionuclides by gas bubbles is also subject to considerable uncertainty. However, cautious scoping calculations designed to provide an upper bound to the possible radiological impacts from this transport mechanism again show these radiological impacts to be insignificant and therefore the uncertainties do not undermine the safety assessment.

6.2.9 Adequacy of references supporting the handling in SR-Site

Since the handling outlined above is based on a geosphere effectively being short circuited, with gas generated at the repository being approximated as moving directly into the biosphere, no supporting references are needed. The motivation for the handling of sorption of colloids on gas bubbles is based on a scientific publication.

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Appendix A

Glossary of abbrevations and specialised terms

This appendix contains explanations to acronyms and technical terms used by SKB that occur in this report.

1D	One dimensional
2D	Two dimensional
3D	Three dimensional
3DEC	Numerical modelling tool for static and dynamic three-dimensional analyses of fractured rock and structural support.
ABAQUS	General-purpose modelling tool for two and three dimensional analyses.
AC	Alternating Current
APSE	Äspö Pillar Stability Experiment
ATP	Adenosin-Tri-Phosphate
Äspö HRL	Äspö Hard Rock Laboratory
BAT	Best Available Technique
BET	Brunauer Emmet Teller; A method for determining the specific surface area of a solid material available for sorption, by use of gas adsorption.
BIFROST	Baseline Inferences for Fennoscandian Rebound, Sea-level, and Tectonics; A project that studies isostatic and other deformations of the Earth's crust in Fennoscandia using available national GPS-stations.
CAPS	Counterforce Applied to Prevent Spalling; experiments conducted at the Äspö HRL to determine if the application of dry bentonite pellets is sufficient to suppress thermally-induced spalling in KBS-3 deposition holes.
CCC	Critical Coagulation Concentration
CFM	Colloid Formation and Migration experiment; conducted at the Grimsel test site
CFT	Colloid-facilitated transport
COMP23	Near-field model calculating the release rate of radionuclides into the geosphere far field.
ConnectFlow	Numerical modelling tool for simulation of groundwater flow.
CPM	Continuous porous medium
CSH, C-S-H	Calcium silicate hydrates
D2	Repository layout adapted to Forsmark site conditions as defined in the site description Forsmark at the completion of the site investigations, SDM Site Forsmark
DarcyTools	Numerical modelling tool for simulation of groundwater flow.
DC	Direct current
DDA	Discontinuous Deformation Analysis
D_e	Effective diffusivity in rock matrix
DEM	Distinct Element Method
Decovalex	DEvelopment of COupled models and their VALidation against Experiments. International cooperation project aimed at the development of THMC modelling techniques.
Deformation zone	Refers to an essentially 2D structure along which there is a concentration of brittle, ductile or combined brittle and ductile deformation. Deformation zones at Forsmark are denoted ZFM followed by two to eight letters or digits.
DFN	Discrete Fracture Network
EBS	Engineered Barrier System
ECPM	Equivalent Continuous Porous Medium
EDZ	Excavation Damaged Zone
EU	European Union
F, F-factor	Transport resistance along flow path [T/L], expressing the relation between flow wetted surface and groundwater flow. It controls retention of radionuclides in the geosphere.
FARF31	Numerical modelling tool for calculation of radionuclide transport in the geosphere
FARF33	Numerical modelling tool for calculation of radionuclide transport in the geosphere which also can handle colloid-facilitated transport
FEM	Finite Element Model
FEP	Feature, Event, Process
FFMxx	Fracture domain at Forsmark; volume of rock outside deformation zones
FHA	Future Human Actions

F_m	Formation factor defined as D_e/D_w where D_e and D_w are effective diffusivity and diffusivity of tritiated water in free water. The formation factor quantifies the reduced diffusion rate obtained in the rock material relative to that in free (unconfined) water.
FPI	Full Perimeter Intersection
GIA	Glacial Isostatic Adjustment
GPS	Global Positioning System
HVDC	High Voltage Direct Current
ISO 9001: 2000	Quality management system standard.
JCS	Joint Compressive Strength
JCR	Joint Roughness Coefficient
KBS-3	KärnBränsleSäkerhet – 3. Method for final disposal of spent nuclear fuel where: the spent nuclear fuel is enclosed in water-tight and load bearing canisters; the canisters are deposited at 400–700 meters depth in crystalline rock; the canisters are surrounded by a buffer preventing groundwater flow and protecting the canister; the rock cavities required to deposit the canisters are backfilled.
K_d	Distribution coefficient for sorption [L^3/T].
LMMOA	Low Molecular Mass Organic Acid
LTDE-SD	Long Term Sorption Diffusion Experiment conducted at the Äspö Hard Rock Laboratory
M, Mw	Earthquake magnitude
M3	Multivariate mixing and mass balance calculation program
MARFA	Migration Analysis of Radionuclides in the Far Field; Numerical modelling tool for calculation of radionuclide transport in a sparsely fractured medium.
MIKE SHE	Numerical modelling tool for surface hydrogeological modelling
Nagra	Nationale Genossenschaft für die Lagerung Radioactiver Abfälle, Switzerland.
NEA	Nuclear Energy Agency
NETPATH	Numerical modelling tool for chemical speciation, batch reaction, one-dimensional transport, and inverse geochemical calculations.
NTP	Normal Temperature and Pressure; denote conditions of 25°C and 1 atmosphere pressure
OPC	Ordinary Portland Cement
PHREEQC	Numerical modelling tool for chemical speciation, batch reaction, one-dimensional transport, and inverse geochemical calculations.
POLY3D	Numerical tool for static three-dimensional analyses of fractures in elastic media.
Q1	Release position for particle tracking; Q1 refers to path starting at fracture intersection with deposition hole.
Q2	Release position for particle tracking; Q2 refers to EDZ path.
Q3	Release position for particle tracking; Q3 refers to path starting at fracture intersection with deposition tunnel.
QA	Quality Assurance
Q_{eq}	Equivalent flow rate; used in COMP23
R&D programme	Research and Development programme
RETROCK	EU project dealing with how retention processes are handled in safety assessment modelling.
SDM	Site-descriptive model
SFR	A repository for low- and intermediate level operational waste at Forsmark
SRB	Sulphate Reducing Bacteria
SSM	Swedish Radiation Safety Authority (Svenska Strålskyddsmyndigheten)
Target volume	The north-western part of the candidate area at Forsmark and the rock volume beneath that has been selected as potentially suitable for hosting a final repository for spent fuel.
TDS	Total Dissolved Solids
TRUE	Tracer Retention Understanding Experiments; experiments conducted at the Äspö HRL.
TSM	Thermodynamic Sorption Model
t_w	Advective travel time
TWI	Topographical Wetness Index
TVO	Teollisuuden Voyma OY; A Finnish electricity generating company owning and operating two nuclear power plant units on the west coast of Finland.
UDEC	Numerical modelling tool for static and dynamic two-dimensional analyses of fractured rock and structural support.
URL	Underground Research Laboratory (in Canada)
ZFMA2	Gently dipping deformation zone at Forsmark
ZFMF1	Gently dipping deformation zone at Forsmark