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Geosphere process report for the safety assessment SR-Can

Svensk Kärnbränslehantering AB

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Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

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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-Can, which is a preparatory step for a safety assessment that will support the licence application for a final repository in Sweden.

The work of compiling this report has been lead 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, 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, Enviros, Spain; Gunnar Gustafsson, Chalmers University of Technology, Sweden; John Hudson, Rock Engineering Consultants, UK; Ivars Neretnieks, Royal Institute of Technology, Sweden; Mike Thorne, Mike Thorne and Associates Ltd, UK; Ari Luukkonen, Nuria Marcos, Petteri Pitkänen, Margit Snellman and Lasse Koskinen, Posiva, Finland; and Per-Eric Ahlström, Olle Olsson and Raymond Munier, SKB.

Stockholm, October 2006

Allan Hedin

Project leader SR-Can

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1 Introduction

1.1 Role of this process report in the SR-Can 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-Can. The detailed assessment methodology, including the role of the process report in the assessment, is described in the SR-Can Main report, /SKB 2006b/. 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 ten steps has been developed for SR-Can, 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-Can FEP catalogue, containing FEPs to be handled in SR-Can, has been established. This step is documented in the SR-Can FEP report /SKB 2006c/.

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 SR-Can Initial state report /SKB 2006h/. The initial state of the geosphere and the biosphere is that of the natural system prior to excavation, as described in the site descriptive models /SKB 2005c, 2006a/. The repository layouts adapted to the sites are provided in underground design reports for each site /Brantberger et al. 2006, Janson et al. 2006/.

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-Can Climate report /SKB 2006e/, 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-Can is described in the SR-Can FHA report /SKB 2006i/.

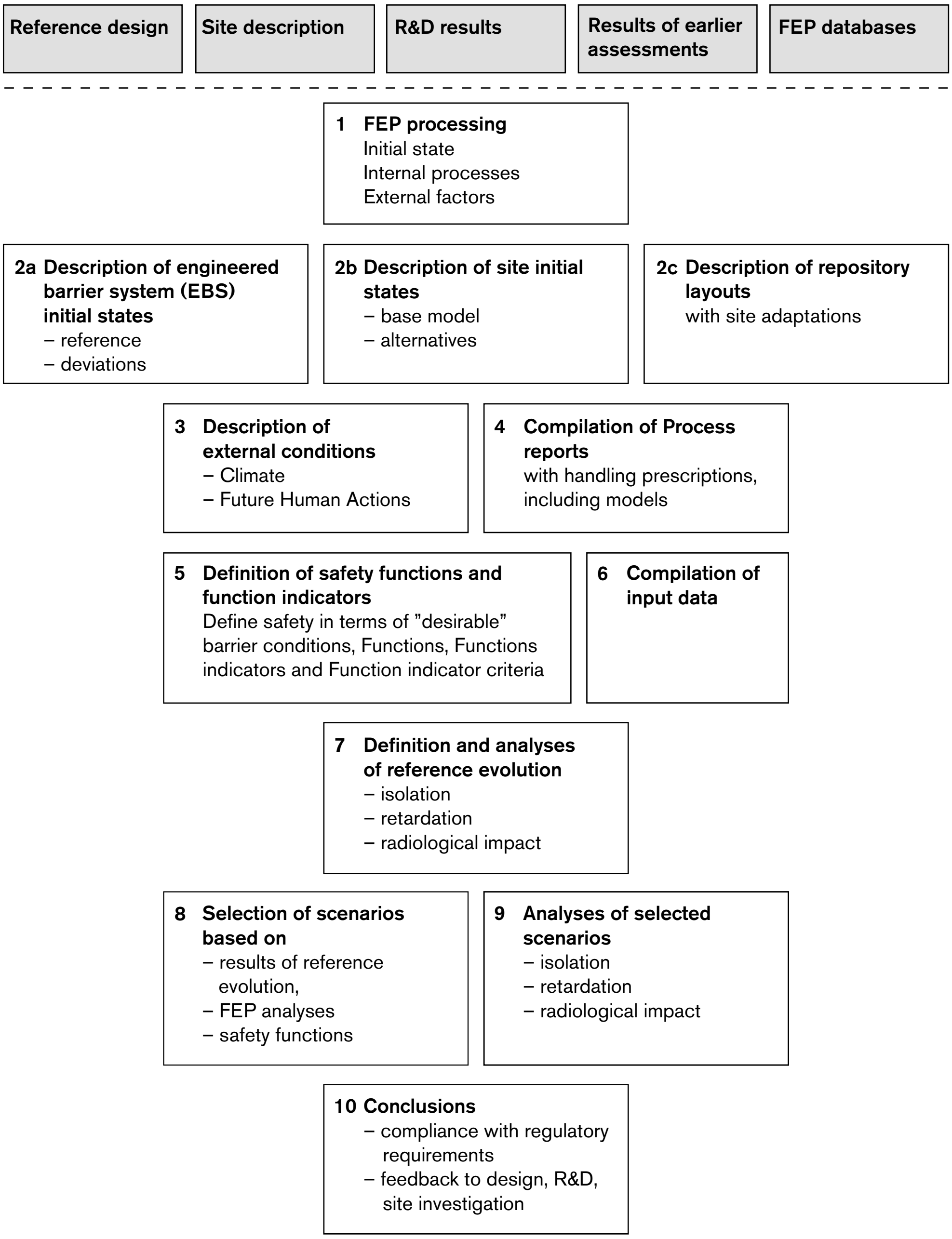


Figure 1-1. *An outline of the ten main steps of the SR-Can safety assessment. The boxes at the top above the dashed line are inputs to the assessment.*

4. Description of processes.

   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 2006f/ and for the buffer and backfill /SKB 2006g/. 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.

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. Input data selection.

   Data to be used in the quantification of repository evolution and in dose calculations are selected using a structured procedure. The process of selection and the data adopted are reported in a dedicated Data report /SKB 2006d/. 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 in a first step, yielding a description of the general system evolution and an evaluation of the safety function indicators. If the evolution indicates breaching of isolation, the retarding potential of the repository and its environs is analysed and dose consequences are calculated for the long-term conditions identified in the first step. Also, some canister failure modes not resulting from the reference evolution are analysed in order to further elucidate the retarding properties of the system. Each process is handled in accordance with the plans outlined in the process reports.

8. Selection of scenarios.

   A set of scenarios for the assessment is selected. A comprehensive main scenario is defined in accordance with SKI's regulations SKIFS 2002:1. 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 4 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 e.g. scenarios explicitly mentioned in applicable regulations, such as 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. An important result is 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 scenario. For these scenarios, as for the main scenario, a risk contribution is estimated.

10. 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 R&D programme.

This Geosphere process report is one of the process reports mentioned in step 4 above. The purpose of the process reports is to document the scientific knowledge of the processes to a level required for an adequate treatment of the processes 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 motivate, by arguments founded on scientific understanding, the treatment of each process in the safety assessment. The purpose is further 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 the SR 97 version of the Process report /SKB 1999/ is a starting point for this SR-Can version. As a result of the FEP processing (step 1 above), the list of relevant processes has been reviewed and slightly extended, see the SR-Can FEP report /SKB 2006c/ for details. Furthermore, the SR 97 process report covering fuel, canister, buffer/backfill and geosphere processes has been replaced by several reports of which the present one covers geosphere processes. A complete list of processes described in the SR-Can process reports can be found in the abovementioned FEP report.

1.1.3 Relation to specific sites

The SR-Can assessment builds on site-specific data and site-descriptive models of the Forsmark area /SKB 2005c/ and the Laxemar subarea /SKB 2006a/, which currently are being investigated as candidate sites for a final repository for spent nuclear fuel in Sweden, see further the SR-Can Main report /SKB 2006c/. Geosphere data for SR-Can are obtained from the site-descriptive model versions 1.2, which are based on the initial site investigation stage. The process descriptions are of a sufficiently general nature to be applicable to both these sites. However, the result of the quantitative evaluations of the processes in the different scenarios analysed in SR-Can will, in many cases, be dependent on site-specific data. These data are not given here, but in dedicated model studies. In addition, the most essential data for the safety assessment are thoroughly evaluated in the SR-Can Data report /SKB 2006d/, 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-Can 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-Can assessment.

1.2 Structure for process descriptions

All identified processes are documented using a template, where many of the headings are the same as those used in the SR 97 report. These are described below.

Overview/general description

Under this heading, a general description of the knowledge regarding the process is given. For most processes, a basis for this is the contents of the SR 97 Process report /SKB 1999/, but 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-Can 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.

Time perspective

The time scale or time scales on which the process occurs are documented, if such timescales can be defined.

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.

Handling in the safety assessment SR-Can

Under this heading, the handling in the safety assessment SR-Can 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.
- 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-Can covers the time span of a Quaternary glacial cycle, that is 120,000 years. Hence, it covers the excavation/operation period, the initial temperate period, and the evolution of permafrost, temperate and glacial periods, following the initial temperate period. It is not possible to predict future climate conditions within this time frame. Instead, the evolution after the initial temperate period is described as a time series of climate domains. These are the temperate, permafrost and glacial domains /SKB 2006e/. In order to reflect different conditions of relevance for repository performance during the assessment period, the following time periods/climate domains are addressed in the descriptions of the handling of the processes:

- Excavation/operation period.
- Initial temperate period.
- Permafrost.
- Glaciation.

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 an event is 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 1.5.

Handling of uncertainties in SR-Can

Given the adopted handling of each process in the safety assessment SR-Can, 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 documentation 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 the 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-Can Data report /SKB 2006d/, to which reference is made if relevant.

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-Can” and “Uncertainties” have been produced by Jan-Olof Selroos (flow and transport processes), Ignasi Puigdomenech (geochemical processes) and Allan Hedin, SKB in collaboration with the expert(s) that assembled the information on the process in question. In addition, Raymond Munier, SKB, and Johan Andersson, JA Streamflow AB, have contributed information that has been included in the mechanical process descriptions. All these experts are included in the SR-Can expert database, see further the SR-Can Main report /SKB 2006b/.

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	Juha Hartikainen, Helsinki University of Technology, Finland; Tomas Wallroth, Bergab AB, Sweden
3.1	Groundwater flow	Peter Jackson, Serco Assurance, UK; Jan-Olof Selroos, SKB, Sweden
3.2	Gas flow/dissolution	William Rodwell, Serco Assurance, UK; Jan-Olof Selroos, SKB, Sweden
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	Surface weathering and erosion	Lena Morén, SKB, Sweden; Jens-Ove Näslund, Stockholm University, Sweden
4.7	Erosion/sedimentation in fractures	Ignasi Puigdomenech, SKB, Sweden
5.2	Advection/mixing	Jan-Olof Selroos, SKB, Sweden; Marcus Laaksoharju, Geopoint AB, Sweden
5.3	Diffusion and matrix diffusion	Kristina Skagius, Kemakta AB, Sweden; John Smellie, Conterra AB, Stockholm, Sweden
5.4	Speciation and sorption	Jan-Olof Selroos, SKB, Sweden
5.5	Reactions groundwater/rock matrix	Eva-Lena Tullborg, Terralogica AB, Sweden; John Semllie, Conterra AB, Sweden.
5.6	Dissolution/precipitation of fracture-filling minerals	Eva-Lena Tullborg, Terralogica AB, Sweden
5.7	Microbial processes	Karsten Pedersen, University of Gothenburg, Sweden
5.8	Degradation of grout	Jorge Molinero, University of Santiago de Compostela, Spain
5.9	Colloid formation and transport	Susanna Wold, Royal Institute of Technology, Sweden
5.10	Formation/dissolution/reaction of gaseous species	William Rodwell, Serco Assurance, UK; Ignasi Puigdomenech, SKB, 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	Ignasi Puigdomenech, SKB, Sweden
6.1	Transport of radionuclides in the water phase	Jan-Olof Selroos, SKB
6.2	Transport of radionuclides in the gas phase	William Rodwell, Serco Assurance, UK; Jan-Olof Selroos, SKB, Sweden

1.4 Definition of the geosphere system and variables

As mentioned in Section 1.1.3, the SR-Can assessment builds on site-specific data and site descriptive models of the Forsmark area and the Laxemar subarea, and the process descriptions in this report are sufficiently general to cover both these sites.

For the purpose of the process descriptions, the geosphere system is defined as the bedrock surrounding 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 in essence the same as those adopted in the process descriptions of the SR 97 assessment /SKB 1999/. 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 preliminary site descriptions of the Forsmark area /SKB 2005c/ and the Laxemar subarea /SKB 2006a/.

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 flow	Gas 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 description of gases in geosphere cavities including any radionuclides.
Structural and stray materials	Chemical composition and quantities of grouts and other structural and stray materials injected/located in fractures in the rock.
Saturation	Degree of water saturation of the geosphere.

1.5 Summary of handling of processes in SR-Can

Table 1-3 summaries the handling of geosphere processes in the safety assessment SR-Can, 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.

Table 1-3. 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. Non-coloured fields denote processes for which basis for definite handling in SR-Can has not been developed.

Process	Excavation/ operation	Temperate	Permafrost	Glaciation	Earthquakes
Ge1 Heat transport	Neglected since sensitivity studies show that time evolution of heating is not sensitive to detailed pattern of deposition.	Modelling of peak canister temperature and temperature distribution in rock.	Site-specific 1-D estimations of permafrost depth.	Site-specific 1-D estimations of sub-glacial permafrost depth.	Not relevant.
Ge2 Freezing	Not relevant.	Not relevant.	Site-specific 1-D estimations of permafrost depth.	Site-specific 1-D estimations of sub-glacial permafrost depth.	Not relevant.
Ge3 Groundwater flow	Modelling of inflow and upconing assuming saturated flow (Darcy Tools). MIKE-SHE for simulating near-surface effects.	Modelling of resaturation (DarcyTools) and saturated flow in different scales (CONNECTFLOW).	Modelling of flow pattern with Darcy Tools.	Modelling of groundwater flow pattern during advance and retreat of an ice sheet.	Not handled in SR-Can.
Ge4 Gas flow/ dissolution	Neglected based on arguments supporting the assumption of small effects of unsaturated regions on inflows to tunnels.	Neglected provided that gas generated in the repository can rapidly escape through the geosphere without causing pressure build-up.	Not handled in SR-Can.	Not handled in SR-Can.	Not relevant.
Ge5 Displacements in intact rock	3DEC stress modelling of near-field effects of excavation of tunnels and deposition holes.	3DEC modelling of thermal stresses and deformations.	Thermal effects neglected provided that only marginal changes in mechanical state occur.	3DEC stress modelling of near 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 construction-induced stresses too limited and expected to be relaxed at the time of deposition.	3DEC modelling of reactivation due to thermal load. Estimation of earthquake probability (consequence analysis, see Earthquake).	Thermal effects neglected provided that only marginal changes in mechanical state occur. Estimation of earthquake probability (consequence analysis, see Earthquake).	3DEC modelling of ice-load induced reactivation. Assessment of MH effects of hydraulic jacking. 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.

Process	**Excavation/ operation**	**Temperate**	**Permafrost**	**Glaciation**	**Earthquakes**
Ge7 Fracturing	Assessment of EDZ. Modelling (3DEC) and observations (APSE) of fracturing around deposition holes (spalling).	Modelling (3DEC) of potential for fracturing induced by thermal stresses. Estimations of effects of gas overpressure.	Thermal effects neglected provided that only marginal changes in mechanical state occur.	Modelling (3DEC) of potential for fracturing induced by ice load. Assessment of risk for hydraulic fracturing.	Neglected based on observations 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 weathering and erosion	Not relevant.	Neglected because of low erosion rates.	Neglected because of low erosion rates.	Neglected because of low erosion rates.	Not relevant.
Ge10 Erosion/ sedimentation in fractures	Neglected because of too low flow rates in non-grouted fractures.	Neglected based on site observations indicating limited significance at repository depth.	Neglected based on site observations indicating limited significance at repository depth.	Neglected based on site observations indicating limited significance at repository depth.	Not relevant.
Ge11 Advection/ mixing	Advection of salt included in hydro-geological modelling. Composition of mixtures assessed from hydrogeological modelling and site understanding.	Advection of salt included in hydro-geological modelling. Composition of mixtures assessed from hydrogeological modelling and site understanding.	Modelling of transport of out-frozen salt.	Modelling of up-coning of saline water and transport of glacial meltwater to repository depth.	Not relevant.
Ge12 Diffusion and matrix diffusion	Diffusion of salt between mobile and immobile groundwater included in hydrogeological modelling.	Diffusion of salt between mobile and immobile groundwater included in hydrogeological modelling.	Diffusion of salt between mobile and immobile groundwater included in modelling of transport of out-frozen salt.	Diffusion of salt included in modelling of groundwater flow pattern during advance and retreat of an ice sheet. Included in modelling of oxygen consumption.	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.	Simplified K_d-approach for modelling sorption of radionuclides. Speciation considered in the selection of K_d.	Simplified K_d-approach for modelling sorption of radionuclides. Speciation considered in the selection of K_d.	Not relevant.
Ge14 Reactions groundwater/ rock matrix	Neglected since reactions are considered to take place at fracture surfaces only.	Neglected because of expected insignificant impact on groundwater composition and matrix porosity.	Neglected because of expected insignificant impact on groundwater composition and matrix porosity.	Included in modelling of oxygen consumption.	Not relevant.
Ge15 Dissolution/ precipitation of fracture-filling minerals	Modelling of mixing (M3) and of reactions (PHREEQC).	Modelling of mixing (M3) and of reactions (PHREEQC).	Not handled, but effects are judged to be less important than effects of e.g. salt exclusion.	Included in modelling of oxygen consumption. Assessment of impact on flow paths of calcite dissolution/ precipitation.	Not relevant.

Process	Excavation/ operation	Temperate	Permafrost	Glaciation	Earthquakes
Ge16 Microbial processes	Mass balance calculations of organic matter and modelling of microbial processes coupled with solute transport and hydrochemical equlibria calculations.	Mass balance calculations of organic matter and modelling of microbial processes coupled with solute transport and hydrochemical equlibria calculations.	Not handled, but effects are judged to be less important than effects of e.g. salt exclusion.	Not handled in SR-Can.	Not relevant.
Ge17 Degradation of grout	Neglected since expected effects will occur during Temperate period.	Generic modelling of effects on chemistry of fractures.	Not specifically handled. Extra-polation of results from Temperate period.	Not specifically handled. Extra-polation of results from Temperate period.	Not relevant.
Ge18 Colloid formation and transport	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.	Not handled in SR-Can.
	Impact on radionuclide transport not relevant because of intact barriers.	Not handled in SR-Can in terms of radionuclide transport.	Not handled in SR-Can in terms of radionuclide transport.	Not handled in SR-Can in terms of radionuclide transport.	
Ge19 Formation/ dissolution/ reaction of gaseous species	Natural gases neglected since concentrations are expected to remain essentially unchanged.	Natural gas neglected since concentrations are expected to remain essentially unchanged.	Natural gas neglected since concentrations are expected to remain essentially unchanged.	Included in modelling of oxygen consumption.	Not relevant.
Ge20 Methane hydrate formation	Not relevant.	Not relevant.	Not handled in SR-Can.	Not handled in SR-Can.	Not relevant.
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, radioactive decay included in integrated modelling (FARF31).	Advection, dispersion, matrix diffusion, sorption, radioactive decay included in integrated modelling (FARF31).	Advection, dispersion, matrix diffusion, sorption, radioactive decay included in integrated modelling (FARF31).	No credit taken for radionuclide retention in the geosphere.
Ge25 Transport of radionuclides in the gas phase	Not relevant since engineered barriers are intact.	Assessed neglecting the geosphere as a barrier.	Assessed neglecting the geosphere as a barrier.	Assessed neglecting the geosphere as a barrier.	Not relevant.

1.6 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 has been carried out. This work is further described in the SR-Can FEP report /SKB 2006c/.

As mentioned above, the FEP processing has led to a minor revision of the list of geosphere processes compared with those treated in earlier assessments.

The FEP processing has also provided lists of project FEPs in the international NEA FEP database version 1.2 that are related to the different geosphere processes. 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-Can 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-Can FEP report /SKB 2006c/ and the handling is also documented in the SKB FEP database.

In general, the results of these checks showed that FEPs were already covered by the process descriptions and included in existing plans for how to handle the process in the SR-Can assessment. In some cases, additional studies have been initiated as a result of the FEP analysis.

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-Can Climate report /SKB 2006e/.

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 7°C and 20°C in Swedish bedrock /Sundberg 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-Can Climate report /SKB 2006e/).

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, 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 and Fälth 2003/. After 100 years, the decay power will have been reduced by about 70 percent. At a repository depth of about 500 m, the thermal perturbation will reach the ground surface a couple of 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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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. Thermal properties for constant T.		Temperate	Output from calculations.
		Permafrost Glaciation	See Temperate above and Climate report /SKB 2006e/.		Permafrost Glaciation	Output from calculations, see also Section 2.2 Freezing and Climate report /SKB 2006e/.
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 Permafrost Glaciation	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.			
		Permafrost Glaciation	See Temperate above and Climate report /SKB 2006e/.			
Gas flow	Yes.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No.	–	–
		Temperate	Influence neglected; little significance.			
		Permafrost Glaciation	See Temperate above and Climate report /SKB 2006e/.			
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.			
		Permafrost Glaciation	Included in permafrost model (Climate report /SKB 2006e/).			
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.			
		Permafrost Glaciation	Influence neglected; little significance.			

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Rock stresses	No.	–	–	No. But indirectly through temperature.		See mechanical processes in Chapter 4.
Matrix minerals	Yes. Determines thermal properties.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No.	–	–
		Temperate	Use of site-specific thermal properties.			
		Permafrost Glaciation	Use of site-specific thermal properties in permafrost model /SKB 2006e/.			
Fracture minerals	Yes. Marginally and locally.	Excavation/ operation	Heat transport neglected (see Section 2.1.7).	No. But indirectly through temperature and groundwater composition.	–	See chemical processes in Chapter 5.
		Temperate	Influence neglected; little significance.			
		Permafrost Glaciation	Influence neglected; little significance. /SKB 2006e/.			
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	Heat transport neglected (see Section 2.1.7).	No. But, indirectly through temperature.	–	–
		Temperate	Influence neglected; little significance.			
		Permafrost Glaciation	See Temperate above and Climate report /SKB 2006e/.			

Temperature; 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. Furthermore, thermal conductivity in rocks and specific heat capacity are weakly temperature dependent. For the Forsmark site rock types, the conductivity decreases by between 6 and 12% per 100°C, and for the Simpevarp rock types by between 1% and 4% /SKB 2005ab/. 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 with temperature by typically 25% per 100°C, but this parameter is relatively unimportant to the maximum temperatures reached in the near-field. In addition, ignoring the increase is conservative. The approximation that is generally made in temperature calculations, namely that the heat transport properties of the rock are temperature-independent, is, therefore, warranted.

Groundwater flow; Heat transport will give rise to temperature gradients and density changes that affect large-scale circulatory water movements /Claesson 1992, Probert 1998/. 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 in comparison with the conductive heat transport that it can be ignored /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. The groundwater pressure cannot have any influence on the heat transport.

Gas 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 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 and Fälth 2003/. For the design limits, the most important geometrical parameter is the distance between neighboring 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 for the rock thermal conductivity and to the rock heat capacity. In particular the heat conductivity is decisive for the determination of the canister spacing in the different rock units. This parameter is extensively measured in the site investigation program and models for the effects of spatial variations are being tested and established /SKB 2005ab, 2006a/.

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 that these materials could 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 contributes to control of the vapour-liquid equilibrium.

2.1.3 Boundary conditions

Influence of the boundaries

Prevailing and past climate conditions, geothermal heat flow, including radiogenic heat production, and the thermal properties of the rock determine initial temperature and temperature gradients (see also Climate-related issues Section 3.1 Development of permafrost in the SR-Can Climate report /SKB 2006e/).The ground surface acts as a cooled boundary, contributing towards reducing the temperatures in the repository. However, the thermal perturbation does not reach the ground surface until long after the temperatures in the repository, e.g. at the canister surfaces, have begun to drop. The maximum temperature in the near field is, therefore, not affected by conditions at the ground surface.

The bentonite buffer transfers the canister thermal power to the rock, and thereby acts 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. After a few weeks, the heat transport properties of the buffer and the canister are therefore without importance for the temperatures in the rock.

The tunnel backfill has a thermal conductivity of about 1.5 W/(m·K) in water-saturated conditions 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. The volume of the tunnels in relation to that of the near field is so small, however, that the effect can be neglected /Hökmark and Fälth 2003/. 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) /Ageskog and Jansson 1998/.

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 gives the thermal energy that is generated during a given period of time. If it is assumed that 5,000 canisters are deposited with an initial power output of 1,700 W each, it is found that a thermal energy of approximately 15 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 the same as 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

At 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, which also make it possible to determine for which assumptions the design criteria will be satisfied.

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 the development of permafrost are described in the SR-Can climate report /SKB 2006e/.

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 thermomechanical analyses, see e.g. /Hakami et al. 1998, Hökmark 1996/.

/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 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 isotropic and that its heat transport properties are independent of the temperature. 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 /Hökmark 1996/. The solution has also been verified by comparison with numerical calculations of the temperature in the far field /Israelsson 1995/. Figure 2-1 shows analytically calculated temperatures at three points in the near field.

The analytical solution, which is based on the superposition principle, can also be used to analyse effects of dividing the repository up into smaller, separate units and effects of performing deposition on several occasions spread out in time. For the first few years after deposition, the analytical solution over-predicts temperatures very close to the walls of the deposition holes by two or three degrees. Alternative solutions, specifically derived to reproduce the evolution at the walls of the deposition holes accurately are found in /Hedin 2004/ and /Hökmark and Fälth 2003/.

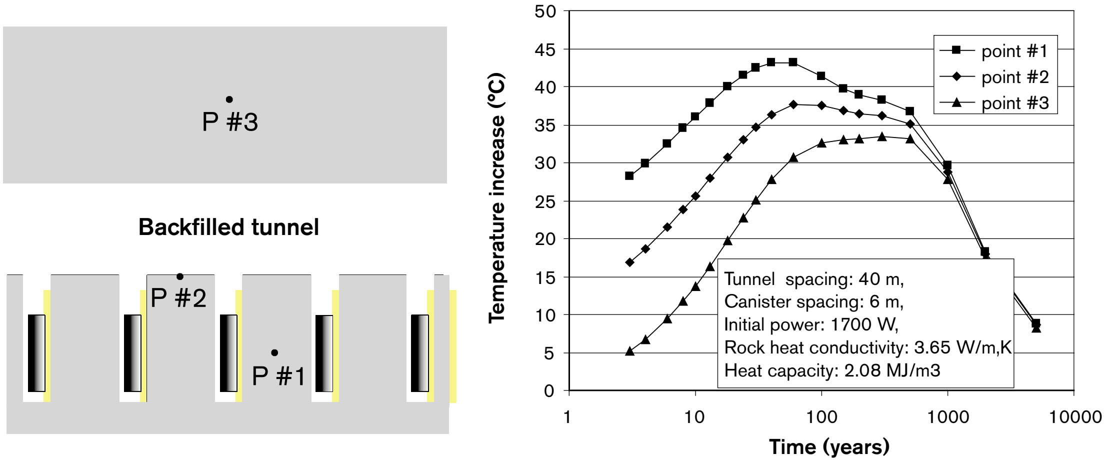


Figure 2-1. *Temperature increase at three points in the near field. The temperatures are calculated using an analytical solution derived by /Claesson and Probert 1996/. Absolute temperatures are obtained by adding the geothermal temperature. Here the repository is modelled as one large rectangular grid of canisters, whereas the real repository will be divided into a number of deposition areas separated by un-heated 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.*

2.1.5 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 and Fälth 2003/. 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 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-isoterm) even 100,000 years after closure, see the SR-Can Climate report /SKB 2006e/.

2.1.6 Natural analogues/observations in nature

Not applicable.

2.1.7 Handling in the safety assessment SR-Can

Excavation/operation period

In the safety analysis, all canisters are assumed to be deposited simultaneously although, in reality, canisters will be deposited at different times. For the near field of a given canister, the only effect of distributing the deposition over time is to offset the local thermal time-scale. For confirmation, the thermal evolution in the near field of an individual canister was modelled assuming deposition to take place tunnel by tunnel with a two year time interval between filling the tunnels /Hökmark and Fälth 2003/. Due to the slow heat propagation and the large (40 m) tunnel spacing, the effects were found to be insignificant. This low sensitivity to details in the deposition pattern is the basis for the assumption of simultaneous deposition and the reason for neglecting heat transport during the excavation/operation period.

Temperate period

The temperature at the walls of deposition holes and the temperature distribution in the rock as function of time after deposition are calculated as a part of the general thermal modelling performed specifically to find the peak canister surface temperature (cf. Buffer and Backfill Process report /SKB 2006g/). 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. 2006/.

Models; The thermal model is described in /Hedin 2004/ and the 3DEC discrete fracture model is described in /Hökmark et al. 2006/.

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, 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.

Permafrost and glaciation

During the one million year assessment time, 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.

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 permafrost and glacial conditions in SR-Can is therefore described in the SR-Can Climate report, Section 3.4 /SKB 2006e/

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-Can

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 about 0.1 W/(m·K) in effective rock heat conductivity at the time of peak canister surface temperature /Hökmark and Fälth 2003/. The nominal decrease is about 0.1% $°C^{-1}$, /Sundberg et al. 2005/, but the increase in rock temperature is high (in the order of 45–50°C) only in small regions close to the deposition holes (cf. Figure 2-1). Neglecting convection is pessimistic and has small effects /Thunvik and Braester 1991/.

Input data and data uncertainties in SR-Can

Input data used in the calculations are compiled and discussed in the SR-Can data report /SKB 2006d/.

Some data uncertainty exists when it comes to effective thermal conductivity and rock heat capacity at the different repository sites /SKB 2005ab, SKB 2006a/. Typical variations in rock heat capacity are not important to the maximum canister surface temperature /Hökmark and Fälth 2003/, whereas variations in rock conductivity may be.

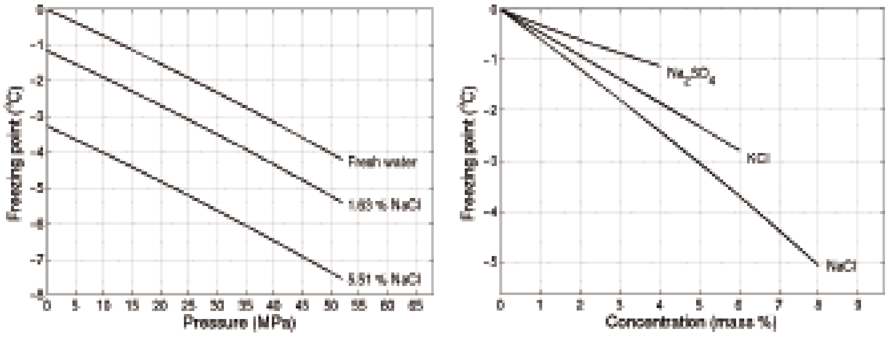
The relevant effective conductivity should be that of rock units with a volume of approximately 30 m × 30 m × 30 m, centered around tunnel sections in which canisters are to be positioned according to the spacing guidelines given in /SKB 2004a/. The rock heat transport properties outside the limits of a volume of that size have little impact on the maximum temperature at the surface of a canister in the central part of the volume. The uncertainty in effective conductivity is related to the way in which the unit is composed of rock types of different conductivities and to statistical variations in conductivity of the different rock types.

2.2 Freezing

2.2.1 Overview/general description

Fresh and unbound 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 have 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 viewed as the process that determines heat transfer in the geosphere, 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 greater 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 transforms the ground to become almost impermeable, thereby reducing the regional groundwater flow and changing the overall groundwater circulation. Exclusion of salts can occur during the freezing of saline groundwater, leading to a redistribution of the salinity concentration around the freezing front (see also Section 5.12). The freezing of in situ water leads to a volume increase of approximately 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, French 1996, Yershov 1998/.



(a) (b)

Figure 2-2. *(a) Pressure-freezing point diagrams for fresh water from /CRC Handbook of Chemistry and Physics 1999/ 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 Handbook of Chemistry and Physics 1999/.*

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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence?	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes.	Permafrost Glaciation.	T from calculations of heat transport (Section 2.1).	Yes. Through the release of latent heat in the freezing process.	Permafrost Glaciation.	Included in models.
Groundwater flow	Yes. But only in highly conductive fractures with large flow.	Permafrost Glaciation.	Neglected; little significance.	Yes.	Permafrost Glaciation.	See Section 3.1 Groundwater flow.
Groundwater pressure	Yes.	Permafrost Glaciation.	Included in models.	Yes. By partial freezing of water in the pore space under over-burden pressure.	Permafrost Glaciation.	Included in the permafrost model.
Gas flow	Yes. But only in highly conductive fractures with large flow.	Permafrost Glaciation.	Neglected; little significance.	Yes.	Permafrost Glaciation.	See Section 3.2 Gas flow/ dissolution.
Repository geometry	No. But indirectly through heat transport and temperature.	–	–	No.	–	–
Fracture geometry	Yes. The amount of freezing water is related to fracture geometry.	Permafrost Glaciation.	Continuum porous medium model adopted. Detailed fracture geometry neglected; low-porosity rocks.	Yes. By volume increase going from liquid to solid state.	Permafrost Glaciation.	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.	Permafrost Glaciation.	Neglected; little significance compared with other influences.	No.	–	–
Groundwater composition	Yes.	Permafrost Glaciation.	Use of site-specific groundwater salinities.	Yes. By exclusion of salt.	Permafrost Glaciation.	See Sections 5.12 and 3.2.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence?	Influence present?	Time period	Handling of influence
Gas composition	Yes. But only when vapour-ice phase change occurs.	Permafrost Glaciation.	Neglected; little significance.	Yes. But only when vapour-ice phase change occurs.	Permafrost Glaciation.	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.	Permafrost Glaciation.	Neglected; assumptions made regarding grout properties in different applications, see Section 5.8.
Saturation	Yes. Affects the amount of freezing water.	Permafrost Glaciation.	Neglected; saturated conditions in the bedrock assumed.	Yes. Degree of saturation decreases.	Permafrost Glaciation.	Neglected; saturated conditions in the bedrock assumed.

Temperature; 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 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 propagation of the freezing front towards greater depths.

Fracture geometry; The amount of freezing water and the adsorptive properties of the porous medium depend on the fracture geometry. 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 ground water pressure through the pore skeleton 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 (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 ground can basically only develop from the ground surface. Hence, a surface temperature below 0 °C is required for freezing of water in the ground. The 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 interannual ground surface temperature can deviate from the air temperature in a range between approximately –1 and +8 °C. In winter, a surface temperature lower than the air temperature can be a 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 air. This means that a mean annual air temperature lower than between –1.5 and –9°C 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. Although, geothermal heat flow is rather steady in time, it is to some extent affected by long-term climate related variations at the Earth's surface, such as the waxing and waining of ice sheets. Geothermal heat flow has a large regional variation in Fennoscandia /Näslund et al. 2005/, which in turn have a substantial effect on the development of perennial freezing of ground (see SR-Can Climate report, Section 3.4 /SKB 2006e/).

Hydraulic boundary conditions

Hydraulic boundary conditions have a direct effect on the freezing process through the groundwater pressure at the freezing point. The major hydraulic effects are due to glacial impacts through the ground surface. The 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 subglacial ground unfrozen. A similar, but more minor, 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 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/. Some recent experimental investigations of thermal, hydrochemical and mechanical impacts of freezing on bedrock properties have been reported by /Kleinberg and Griffin 2005, Ruskeeniemi et al. 2002, Ruskeeniemi et al. 2004, Wegmann et al. 1998/, 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 /Hartikainen 2004, SKB 2006e/.

2.2.5 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 2-3.

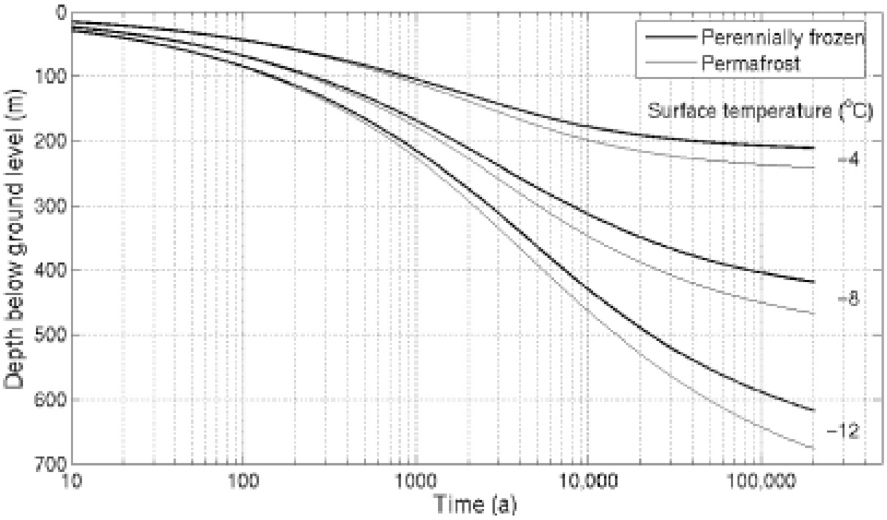


Figure 2-3. *Evolution of permafrost (0°C-isotherm) depth and perennially frozen ground depth for constant ground surface temperatures of –4, –8 and –12 °C at the Forsmark site with present-day mean characteristics, after /SKB 2006e/.*

2.2.6 Natural analogues/observations in nature

Freezing of water in the geosphere is a common feature in boreal and arctic climates. 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 cold-based glaciers.

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

2.2.7 Handling in the safety assessment SR-Can

Temperate, permafrost and glacial 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, permafrost and glacial climate regimes, are estimated by the use of 1-D models. These are based on present day site-specific characteristics and initial conditions. Surface boundary conditions for a reference glacial cycle are produced by the ice sheet model, while colder surface boundary conditions are specified by modifying the reference glacial cycle conditions according to relevant climate scenarios, see SR-Can Climate report, Section 3.4 /SKB 2006e/.

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

Figure 2-4. Permafrost distribution of the ice-free land area in the northern hemisphere, from /International Permafrost Association 1998/.

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 exclusion of salts in freezing of groundwater and the geochemical weathering of the geosphere due to freezing and thawing processes are not yet well-founded.

Model simplification uncertainties in SR-Can

The major model simplification is to carry out the studies in 1-D excluding implications from lateral variations in physical properties, boundary conditions and geometry. Additional simplifications are the continuum approach for the modelling of groundwater flow and neglect of salinity transport. However, both the Forsmark and Laxemar sites are largely composed of relatively low-porosity and low-permeability bedrock, in which case the groundwater flow and salinity of groundwater have minor effects on permafrost development.

Input data and data uncertainties in SR-Can

The reference glacial cycle surface boundary conditions, produced by the ice sheet model 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. Instead, the reference evolution is accompanied by other climate variants, together covering the full range of possible future climate variations within the time frame of a glacial cycle.

Some data uncertainty exists when it comes to effective thermal conductivity and heat capacity of the rock at the different sites, see Section 2.1 and the SR-Can Data report /SKB 2006d/. Thermal conductivity is the most important input parameter of the physical properties that go into the calculation of ground temperature and the rate of freezing.

Some uncertainty also exists in determination of hydraulic and mechanical properties of bedrock and salinity concentrations of groundwater versus depth at the suggested repository sites /SKB 2005c, 2006a/.

The in situ ground temperature has been measured in boreholes down to depths of 500–1,400 m. Between different boreholes the temperature at a specific depth varies over a range of 2°C /SKB 2005ab/. A considerable uncertainty is associated with the method used to estimate the in situ temperature as well as the geothermal heat flow in the 1,000–10,000 m depth range for the initial temperature condition and the bottom thermal boundary condition of the model. The method is based on a stationary heat conduction model with a palaeoclimatically corrected surface geothermal heat flux and a mean surface temperature over a glacial cycle (SR-Can Climate report, Section 3.4 /SKB 2006e/).

Along with the temperature, the freezing process is affected by the water pressure and salinity concentration which, in turn, are dependent on groundwater flow and several chemical processes and their interactions. The data uncertainties related to these processes are described in Section 3.1 and Chapter 5, respectively.

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 rocks and soils, which are generally very small (but may be very large in rocks such as limestones). The voids may include microscopic pores in the rock matrix and fractures. Groundwater and its behaviour are described in many standard textbooks such as /Bear 1972, Freeze and Cherry 1979, de Marsily 1986, Domenico and Schwartz 1998/. Groundwater and its flow play key roles in the performance of a repository for radioactive waste. In the event of radionuclide release from the repository, the groundwater flow determines 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.

At depth, the voids in the rocks generally contain only groundwater – the rocks are said to be saturated. Near the surface, there is generally a region where some of the voids contain air – the rocks are 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 (see Figure 3-1).

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 (see Figure 3-1).

The hydrologic cycle

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

- Water evaporates from seas, lakes, rivers, streams, marshes, 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.

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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 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.

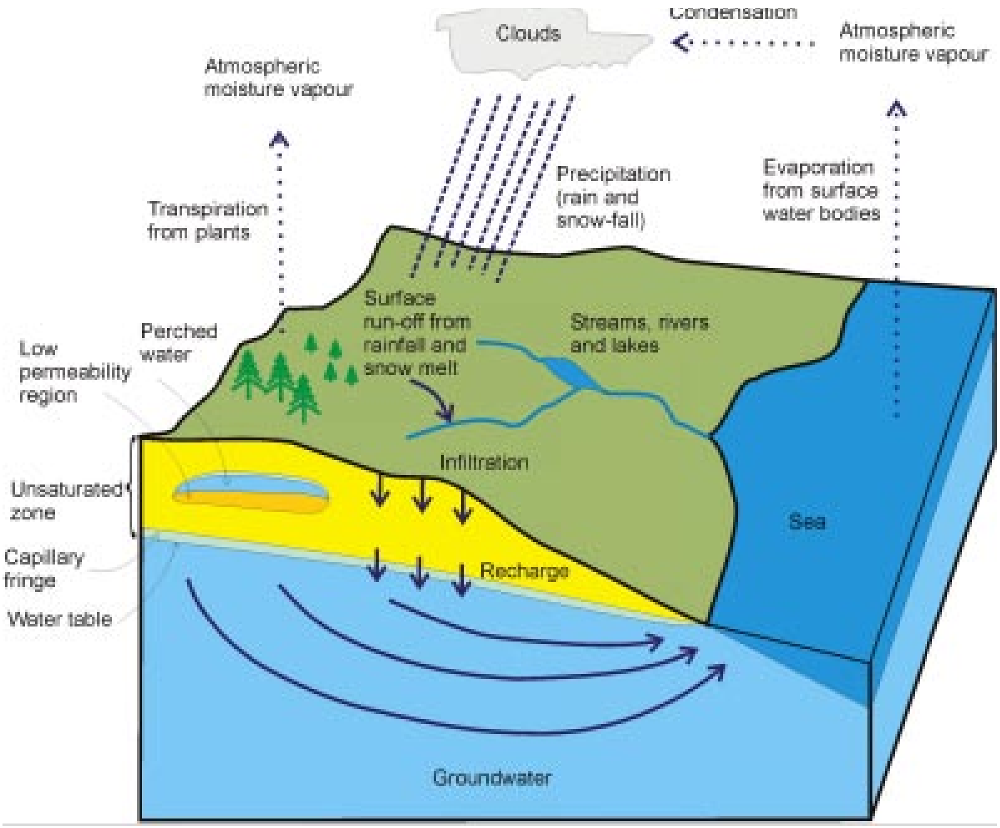

Figure 3-1. *Simplified schematic of subsurface and surface water.*

- 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.

Beneath the water table, groundwater flows through the ground, ultimately discharging where the water table comes to the surface (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.

Driving forces

Groundwater flow is driven by gravity and by gradients in groundwater pressure. The flow is proportional to the driving force, 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 driving force is proportional to the groundwater density.

Groundwater properties

For conditions relevant to a radioactive-waste 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

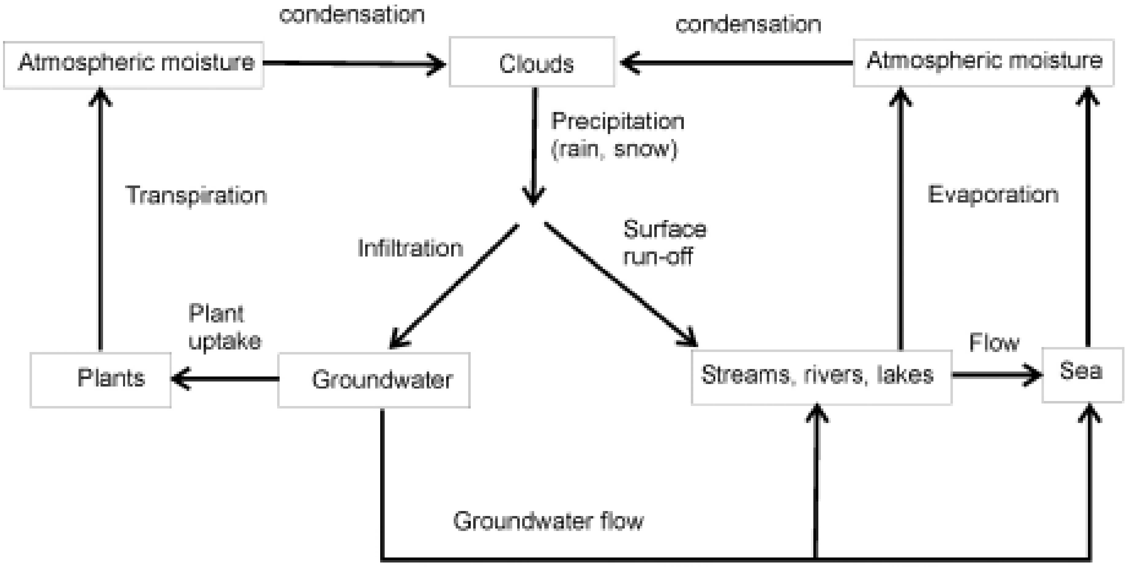

***Figure 3-2.** The hydrologic cycle in simplified form.*

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 2km 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 has a maximum at 4°C.

Modelling of groundwater flow

There are two main types of groundwater flow model: continuum 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, 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 are more detailed and more realistic, in that they represent the flow as being through discrete features, as is considered to be the case physically, and further the models attempt to represent aspects of the features through which there is flow.

Nevertheless, the overall flow on suitable length scales (longer than those of the fractures) can be modelled (to a good approximation) using CPM models /Jackson et al. 2000, La Pointe et al. 1995, Svensson and Ferry 2004/. In the SKB programme, heterogeneous CPM models that represent fractured rocks are referred to as Equivalent Porous Medium (EPM) 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 **q** (the volumetric flux of groundwater through unit area, m·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

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 due to gravity (m·s^{-2})

The permeability is a geometric property of 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. It is usually heterogeneous, that is varies from point to point, typically over several orders of magnitude.

At high flow velocities, which only occur near open boreholes and tunnels, the flow 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 velocities, and to turbulence at very high flow velocities /Scheidegger 1956, de Marsily 1986/. The flow may also be less than that predicted by Darcy's law in compact clays.

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). 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

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

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 ($m^{-2} \cdot s^{-2}$)

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.

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 is 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.

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.

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 a substantial unsaturated zone above the repository. 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 5.1.) 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 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 /Hartley et al. 2005ab, Rhén and Smellie 2003/ 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 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 /Hartley et al. 2004/

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

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

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 presentating 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 and Wallin 1997/.

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

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

where

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

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

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

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

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

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 plus the gravitational force, 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 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 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 regional- and local-scale models, which separately contain a number of finite elements near the limits for practicable calculations, will be used. 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 elements, 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 Laxemar and Forsmark, 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, 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 CPM and DFN representations, or a combination, may be used for this.

It is possible that models on different scales may be nested, 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.

Effective properties, upscaling and DarcyTools

CPM models require values of the permeabilities for the elements (or grid blocks). For blocks corresponding to fractured rocks, these values may be obtained by a process of upscaling from the underlying fracture network. The fracture network in a block is modelled. The flow through the block is calculated for a given pressure difference across the block in a given direction. The effective permeability for the block is then the permeability of a homogeneous block in a CPM model that would give the same overall flow through the block. The effective permeability represents the effect of the fractures within the block.

The program DarcyTools /Svensson and Ferry 2004/ uses a CPM approach for modelling fractured rocks, but the effective permeability of a grid block is obtained by a slightly different upscaling approach to that described above. Darcy Tools is based on the view that the transmissivity of the fractures is correlated with their size, with smaller fractures being less transmissive, so that even though there are many more small fractures than large ones in a volume of rock, the flow is predominantly through larger fractures and large-scale features. The fractures and large-scale features are taken to have a fractal power-law size distribution with the density of fractures increasing with decreasing fracture size.

In DarcyTools, the upscaled flow properties for a grid block representing a fractured rock are not obtained by explicit flow calculations for the block. Instead, the effective properties for a grid block are calculated directly as the sum of contributions from the large-scale features and fractures that cross the grid block. Darcy Tools 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 effective hydraulic conductivity. The contribution from a fracture (or feature) to the hydraulic conductivity in a particular direction is essentially given by the conductivity of the fracture multiplied by the fraction of the grid block associated with flow in the particular direction occupied by the fracture. Here the conductivity of the fracture is given by its transmissivity divided by its thickness. This process generally leads to an effective hydraulic conductivity that is heterogeneous and anisotropic, noting that the grid blocks associated with flow in different direction are different.

It can be shown that the approach used in Darcy Tools gives a good representation for fractures and features with length scales comparable to, or larger than, the size of the grid block /Svensson 2004/. The smaller fractures are not neglected. Their volume is taken to contribute to the volume of immobile water available for rock-matrix diffusion. A similar approach is used to calculate the effective porosity of a grid block and the flow-wetted surface from the contributions from the large-scale features and larger fractures crossing a grid block.

The realism of this approach depends on the parameters of the system. If the fracture density is high, and the density of fractures does not increase very rapidly with decreasing size, and the transmissivity of fractures does not fall off rapidly with decreasing size, then even quite small fractures may be connected and contribute to the flow, and also to the flow-wetted surface. The grid blocks in the modelling should be sufficiently small that most of the fractures that contribute to the flow are taken into account in the calculation of the effective hydraulic conductivity (and flow-wetted surface) for a block.

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

The key properties of the rocks that control groundwater flow are the permeability for a rock in which groundwater flows through pores in the rock matrix, or the transmissivity and connectivity of the fractures for a rock in which groundwater flows predominantly through fractures. The latter rocks may also be modelled by CPM models that represent implicitly the network of fractures carrying the flow. In such models, the permeability is an effective property that represents the effects of the fractures.

As noted previously, the permeability is a tensor, which is generally anisotropic. Rocks are generally very heterogeneous – the permeability varies from point to point, typically over several orders of magnitude.

The transmissivity of a fracture is analogous to the hydraulic conductivity 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 a much greater fracture density 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 highly 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 stress changes or because of precipitation or dissolution of minerals within the fracture. The effective stress on a fracture is the difference between the stress in the rock and the compressive stress corresponding to the pressure in the groundwater. At depth, it is dominated by the stress in the rock. Over time this may change. The main process leading to stress changes on the timescales of interest is the load resulting from the presence of ice sheets during glacial periods. The stress may also change because of tectonic changes (which are very slow), earthquakes, as a result of the construction of a repository, or because of temperature changes due to the heat given out by a repository.

If there is an increase in the compressive stress normal to a fracture, then the fracture will tend to close, decreasing its transmissivity. The transmissivity will generally be related to the compressive stress in a complicated way because the opposite surfaces of the fracture are only in contact over a relatively small part of the fracture surface. 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 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). 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 the rock adjacent to the tunnel will be altered. 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. However, even in the latter case, the zone in question is only tens of centimetres thick /Emsley et al. 1997/. In the EDZ, additional fractures may be created and existing fractures may extend and/or change their aperture, leading to changes in transmissivity.

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 effects the flow through its impact on rock-matrix diffusion of salinity, may also be affected by precipitation and dissolution.

The impact of such processes will be largest in the very near-surface zone where chemical weathering takes place. Physical and biological weathering will also take place in this zone. However, the impact of the weathered zone on the flow in the deep rocks is likely to be small.

As well as the properties of the rocks around the repository, the properties of the tunnels (and shafts) of the repository will also affect the groundwater flow, particularly in the immediate vicinity of the repository. The tunnels would be backfilled before repository closure, but at some potential sites may be slightly more permeable than the original rock, and the backfill might degrade over time and become slightly more permeable. Seals would be placed at selected locations within the tunnels. Provided that these remained effective, they should prevent the tunnels acting as connected paths for flow over their whole length. However, the section of tunnels between seals might still act to connect the more transmissive fractures. Over very long times, seals might fail so that the repository might connect fractures over longer distances. However, the effect of the tunnels and seals on the flow overall is expected to be fairly small.

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 low. Consequently, groundwater tends to build up to elevations where it can be discharged as runoff within the surface hydrological systems.

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 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 features, such as fracture zones or faults. These generally lead to the flow cells related to topography being broken up into smaller local flow cells.

Typically the groundwater salinity increases with depth, with a region of nearly fresh water near the ground surface. 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 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, if the density gradient is large enough, density increasing with increasing elevation is an unstable condition and convection cells will form.

As noted above, the temperature is not significantly affected by the groundwater flow but is predominantly controlled by conduction (see Section 2), 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.

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. This 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-Can Climate report /SKB 2006e/. 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, permafrost* and *glacial domains* /SKB 2006e/. 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 2006e/ 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 2004bc, 2005a/.

Periods of temperate domain are typical for 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 rise of 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 2006e/).

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. As the water freezes 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 permafrost domain and the development of permafrost is further described in the Climate report /SKB 2006e/.

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 frontal-near areas, 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-Can Climate report, Section 3.2 /SKB 2006e/.

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 also extend 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 a 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 discussed in more detail in the SR-Can FHA report /SKB 2006i/.

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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 ground-water, 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 period	Effect of geothermal gradient on density and viscosity considered in main calculations. Impact of thermal effects from waste addressed in scoping calculations.		Temperate period	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.
		Permafrost	Effect of geothermal gradient taken into account. Constant temperature distribution in time because effect of variations over time secondary to effect of permafrost.		Permafrost	Neglected; the effect is small.
		Glaciation	Neglected; secondary to effect of ice sheet.		Glaciation	Neglected; the effect is small.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 flow	Yes. Groundwater flow and gas flow are coupled.	Excavation/ operation/ resaturation	Neglected in calculations of inflow to tunnels; no gas generated by repository and a model representing the water table by a free surface can give the drawdown and inflow.	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.
		Temperate period	Neglected in main flow calculations; small volume of gas generated and effects localized. Impact of gas assessed by scoping calculations.		Temperate period	Considered in estimates of the capacity for transport of dissolved gas. See Section 3.2 Gas flow/dissolution.
		Permafrost	Neglected; effect secondary to effect of permafrost.		Permafrost	Neglected; gas flow is a relatively minor process.
		Glaciation	Neglected; secondary to effect of ice sheet.		Glaciation	Neglected; gas flow is a relatively minor process.
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 period	A detailed representation of repository tunnels included in local flow model.			
		Permafrost	Neglected; effect secondary to other effects addressed (e.g. salt rejection).			
		Glaciation	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.	–	Indirect changes resulting from precipitation/ dissolution not addressed because they are expected to be long-term and relatively very small.
		Temperate period	Site-specific descriptions of geometry of fractures and fracture zones. Impact of EDZ by assigning elevated hydraulic conductivity relative to the host rock. Changes over time neglected; small and within the uncertainties.			
		Permafrost Glaciation	Continuum models based on site-specific descriptions of geometry of fractures and fracture zones.			
Rock stresses	No. But indirectly through changes in fracture geometry.		Not addressed, but stress changes are expected to be relatively small, apart from changes due to ice-loading, repository construction, tectonic changes on very long times and earthquakes.	No. Water flow does not affect stress conditions in rock.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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.
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 and meteoric water by advection and matrix diffusion is modelled.
		Temperate period	Site-specific variations in and distribution of salinity accounted for in the models.		Temperate period	Transport of salinity by advection and matrix diffusion is modelled.
		Permafrost Glaciation	Site-specific salinity effects considered.		Permafrost 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 and the impact on the flow would be very small.
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 period	Grouting is, pessimistically, not represented.		Temperate period	Neglected; see Section 5.8
		Permafrost Glaciation	Pessimistically neglected.		Permafrost Glaciation	Not handled; see Section 5.8
Saturation	Yes. Affects permeability and thus flow	Excavation/ operation/ resaturation	Neglected in calculations of drawdown and inflows to the repository; little significance (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 period	Neglected; saturated conditions in the bedrock.		Temperate period	Neglected; saturated conditions in the bedrock.
		Permafrost	Neglected; the ground would generally be saturated beneath the permafrost (unless a sufficiently large gas bubble forms).		Permafrost	Neglected; the ground would generally be saturated beneath the permafrost (unless a sufficiently large gas bubble forms).
		Glaciation	Neglected; effects secondary to the effects of an ice sheet.		Glaciation	Neglected; effects secondary to the effects of an ice sheet.

3.1.3 Boundary conditions

Numerical simulations of the groundwater flow will be carried out on several scales. Suitable boundary conditions for all the simulations will be needed. The domain for the largest-scale (regional) model is normally 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). 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.

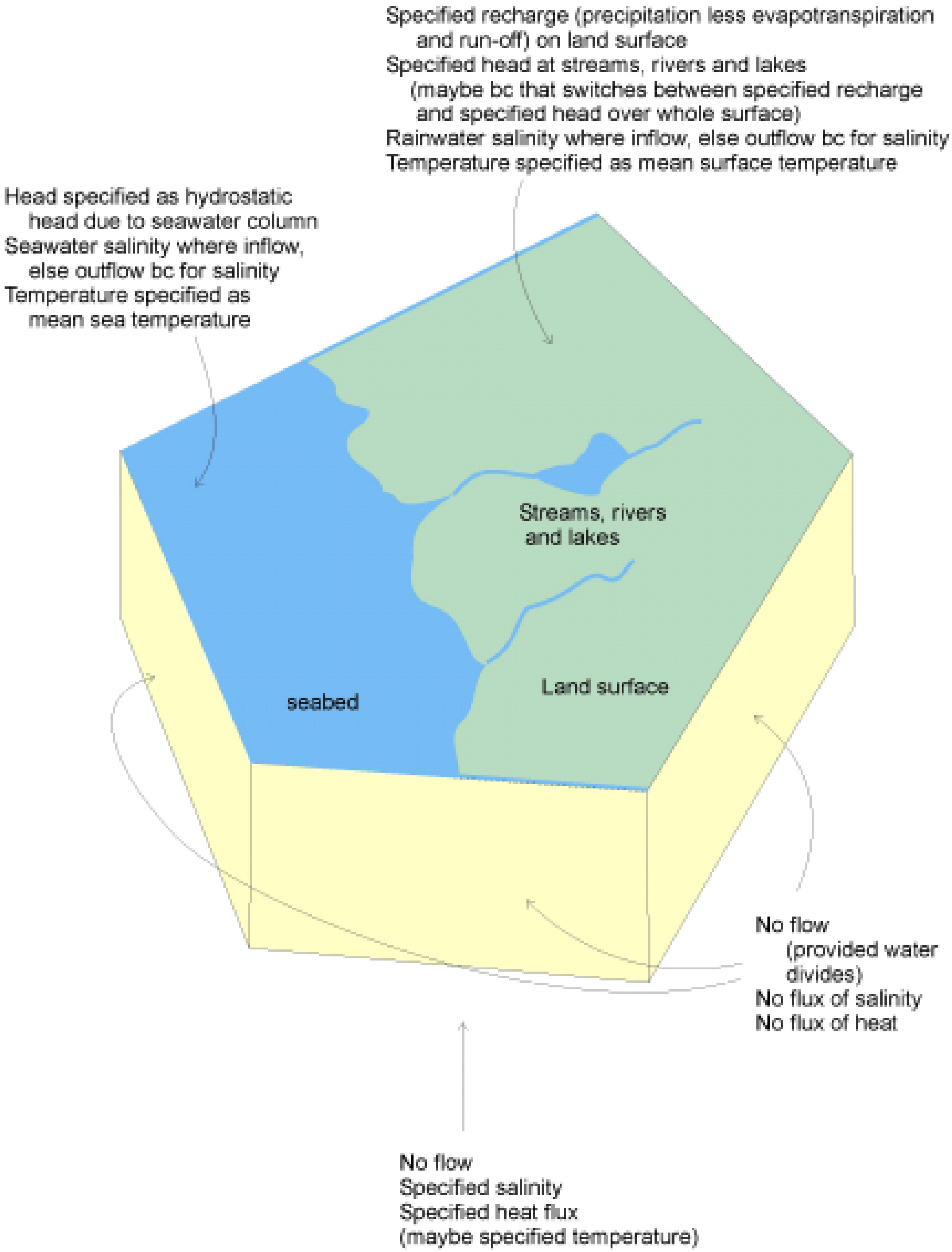

Figure 3-3. Boundary conditions for a regional model.

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 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 time-scales 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. Therefore, it is a reasonable approximation to take the whole of the model to be saturated, that is to neglect the effect of the unsaturated zone, which is normally thin. However, it may be necessary to address the unsaturated zone in modelling groundwater flow during repository construction, when there may be considerable drawdown of the water table in the vicinity of the repository. Except for this context, it is a reasonable approximation for the top-surface boundary condition onshore to take the water table to be at the land surface.

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. The surface elevation changes, which may affect the regions of recharge and discharge. The combined effect of the changing surface elevation with 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 /Boulton et al. 2001, SKB 2006e/.

The discussion above has addressed the boundary conditions for regional models, which are usually based directly on physics. 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 programs (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, Olsson 1992/, 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 Stripa, 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 1997ab, Andersson et al. 2002ab, Poteri et al. 2002, Winberg et al. 2002, Rhén and Smellie 2003/.

Additional insight concerning recharge and discharge patterns for groundwater flow has been gained in recent modelling studies /Holmén et al. 2003, Follin and Svensson 2003/. 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 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 2004/. 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.

3.1.5 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. Therefore, the discussion hereafter will only address 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 being investigated is currently close to the surface and the salinity at depth is approximately horizontally stratified /SKB 2005ac, 2006a/.

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. If the repository is close to the coast, 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. 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/). If the distribution of salinity is perturbed by the site investigation and repository construction, it is not clear how long it might take for the distribution to return to one similar to the original.

A repository will also be a source of heat due to radioactive decay of the waste. 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 the 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'.

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 the temperate, permafrost and glacial domains during the assessment period. If the emission of greenhouse gases perturbes the pattern of glaciations seen in the past, either an extremely long temperate period can be expected in Fennoscandia, or a colder period could start relatively early /SKB 2006e/. The result depends on which associated changes takes place in the North Atlantic Ocean circulation. However, over the full assessment period, phases of permafrost and glacial domain will most probably also occur in a Greenhouse warming scenario.

3.1.6 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 2004bc, 2005ac, 2006a/. 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.

3.1.7 Handling in the safety assessment SR-Can

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

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 DarcyTools program /Svensson et al. 2004, Svensson and Ferry 2004, Svensson 2004/. The calculations use a saturated groundwater flow model, with the water table represented by a free surface. (DarcyTools could also model the unsaturated flow above the water table using an approximation.) Additional simulations of near-surface effects are carried out using the hydrogeological modelling tool MIKE-SHE /DHI 2003/ 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 2005c, 2006a/ and the tunnel layouts /Brantberger et al. 2006, Janson et al. 2006/.

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 may be necessary.

Temperate period

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. The calculations use a combination of DFN, EPM and CPM models on a range of scales. Regional-scale EPM and/or CPM models are used. Major transmissive features in the region and the backfilled tunnels are represented explicitly.

The permeabilities of blocks of fractured rock within the 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 EPM 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 nested within the repository scale models. Thus, an explicit CPM representation of the repository tunnels and the deposition holes is nested in the repository scale models.

The calculations are undertaken using the program CONNECTFLOW. The modelling is illustrated by the simulations carried out for the SR-Can Interim Assessment /Hartley et al. 2004/.

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 2005c, 2006a/, and the tunnel layouts /Brantberger et al. 2006, Janson et al. 2006/.

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. These effects are addressed by scoping calculations.

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 are carried out to address this issue.

Permafrost

In the SR-Can 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. Calculations are also carried out to examine the movement of saltwater arising from salt exclusion during freezing beneath an advancing permafrost front.

The DarcyTools code is used for these simulations. The main input to the simulations is the site-descriptive models /SKB 2005c, 2006a/. Information on the potential extent of permafrost is also required to help identify suitable schematic calculations.

Glaciation

Calculations are carried out to examine the groundwater flow patterns during the advance and retreat of an ice sheet. The calculations are undertaken with a model covering an even larger domain than the regional model. The configuration of the sub-glacial hydrological system is based on studies of glaciers and the Greenland ice sheet. The movement of the ice sheet, its thickness, basal conditions and melt-water production are obtained from an ice-sheet model /SKB 2006e/.

The program CONNECTFLOW is used for the calculations. The main inputs to the calculations are the site-descriptive models /SKB 2005c, 2006a/, the configuration of the sub-glacial hydrology and information about the ice sheet obtained from an ice-sheet model, see SR-Can Climate report /SKB 2006e/.

Earthquakes

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

3.1.8 Uncertainties

There are various uncertainties associated with the groundwater flow system over the periods to be considered.

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.

Parameter uncertainties

Even though there may only be small conceptual and implementation uncertainties about the models for groundwater flow, there are considerable uncertainties about the parameters for these models. Rocks are highly heterogeneous and contain many features (such as major transmissive zones), which are also highly heterogeneous. Therefore, it is not possible to characterise the detailed variation of the rock properties within a region of interest with a finite investigation programme. In practice, all that can be done is to characterise the variability statistically on the basis of available measurements. There will still be uncertainty. There is uncertainty about the appropriate statistical model as well as about the parameter values characterising a particular model. (For example, a particular quantity might be represented by a log-normal distribution or by a beta distribution, or a power law distribution, cf the fracture density in Darcy Tools). Such uncertainties may be addressed by considering alternative models. For a particular statistical model, there will be uncertainty about its parameters, because the number of measurements that can be made is finite. The site investigation programme will try to obtain sufficiently many measurements at suitably distributed locations to reduce the uncertainties to acceptable levels. A large number of measurements may be required. There is also uncertainty resulting from a particular statistical model with identified parameters. This can be addressed by considering a number of realisations (or examples) of the model. There are particular uncertainties about major features. Even though the positions and properties of these are well characterised within certain well-investigated volumes of rock, there are considerable uncertainties about the positions and properties of such features elsewhere in the region of interest.

There is considerable uncertainty about the network of conductive features. The relationship between geologically interpreted structures and hydraulic structures is not clear cut. There are also uncertainties about the connectivity of features and fractures on a large scale, and it is only possible to obtain limited information about this. For example, cross-hole tests may provide some information about the connectivity of the more permeable features.

The models developed can be tested by comparing the results of model calculations with experimental observations, such as measurements of groundwater head or geochemical measurements of groundwater composition. This may help to reduce the uncertainties by constraining the models.

One particular source of uncertainty arises because experimental measurements provide information on particular length scales. A measurement combines information from length scales smaller than that of the measurement. For example, in a fractured rock, a borehole test effectively combines information about the transmissivities of all the fractures within some region of the tested interval, with greater weight placed on the transmissivities of fractures crossing the interval, and on the parts of these fractures closest to the borehole. The size of the region depends on the duration of the test. In consequence, the test does not uniquely constrain the transmissivity of a single fracture at a point. In order to infer the constraints on such quantities from the measurement, it is necessary to undertake a process of 'down-scaling' on the basis of the models for the distribution of transmissive features and the variation of transmissivity over them. It is then possible to up-scale to the length scales of the parameters that appear in the numerical models.

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.

The power-law size distribution is central to the approach adopted in Darcy Tools. The results of calculations may be very sensitive to the estimated exponent of the model and to the cut-off below which fractures are treated as part of the matrix. Similarly CONNECTFLOW DFN models may be sensitive to the estimated parameters of the DFN models used. Such sensitivities can be addressed through sensitivity calculations. In Darcy Tools, it is an underlying assumption that there is a correlation between fracture transmissivity and size. Although this is considered reasonable, nevertheless there is uncertainty about the model.

There are considerable uncertainties about the parameters for ice sheet models, see The SR-Can Climate report /SKB 2006e/. 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.

Model simplification uncertainties in SR-Can

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

The unsaturated zone is not generally modelled, although a simplified approximation to the unsaturated zone may be used in the DarcyTools modelling of the region above the water table in the calculations for the excavation, operation and resaturation period. Neglect of the unsaturated zone is considered to be a minor approximation in general, because the water 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. However, the study by /Painter and Sun 2005/ showed that a saturated flow model gave good results for the far-field flow and the inflows to the tunnels in this case.

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 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 CONNECTFLOW 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 CONNECTFLOW modelling 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. In the Darcy Tools modelling, the underlying fractures are taken to be rectangular features, without internal structure, so the models do not represent the details of the channelling. However, it is judged that the CONNECTFLOW and Darcy Tools models capture the essence of the fracture flow system.

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-Can

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 2006e/.

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

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).

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. 1999/. In some environments, but not those generally considered suitable for radioactive waste repositories, it has been argued that natural movement of a free gas phase occurs at depths well below the water table. The origin of natural gases in the geosphere is briefly discussed in Section 5.10.

Repository processes that are expected to generate gases include water radiolysis and metal corrosion. Both these processes produce hydrogen. In a Swedish repository for spent fuel, the generation of hydrogen by anoxic corrosion of iron can occur only in the unlikely event that a 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 water radiolysis and canister processes for iron corrosion /SKB 2006f/, and buffer processes and backfill processes for rock bolt corrosion /SKB 2006g/.

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 prevailing hydrostatic value. An increasing quantity of this gas will also dissolve in the groundwater as the pressure rises on resaturation (see below).

Calculations by /Painter and Sun 2005/ based on generic site data showed 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]. That is, an unsaturated zone would be created between the repository and the surface. This would result in the presence of a larger volume of gas in the host rock than that simply from desaturation of the rock close to the repository. However, the gas in the unsaturated zone would remain connected to the surface on repository closure and so much of the gas would be expected to be displaced by resaturating water (although there may also be a significant amount of gas trapped by the imbibing water). The rock permeability assumed by /Painter and Sun 2005/ was significantly higher than that currently indicated at Forsmark, and the infiltration rate significantly lower, so it may be that at the Forsmark site the water table lowering caused by repository operations would not be as great as estimated for the generic site.

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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 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

Gas that remains in solution in groundwater is not considered to have any particular consequences for repository performance that are peculiar to the fact that it 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 2006g/. Earlier work indicated that escape through the host rock of gases generated in waste canisters should occur with no build up of gas pressure /Wikramaratna et al. 1993/, but this needs to be confirmed for site-specific data.

A migrating free gas phase may include radioactive, toxic, or flammable gases, and transport of these to the surface in the gas stream and release there may lead to human exposure to radiation or 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. First, by the collapsing and reforming of gas pathways; second, by the entrainment of groundwater in streams of bubbles. Further discussion and references can be found in /Rodwell et al. 1999/. 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, but no clear demonstrations of these effects in the field, or their quantification, are available.

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 also discussed in Section 5.10.

Gas flow/transport of dissolved gas

Free gas generated in defective waste 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 restricts gas entry. Throughout its migration path 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 "sees" and how close the dissolved gas concentration in this groundwater is to being saturated.

The approach described in Section 3.1 for modelling groundwater flow using Darcy's law is generalised to two phase gas-water flow by the introduction of terms into the equation to take account of the interactions between the two phases, as described in the following paragraphs. 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 Darcy velocity vector, $\mathbf{q}_f$, for phase f is given by:

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

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:

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

where p_c is the capillary pressure.

The terms added to the single-phase Darcy equation to take account of the interactions between the two phases are the relative permeabilities and the capillary pressure, both of which are functions of the gas saturation, the fraction of the pore volume occupied by gas.

As indicated, the capillary pressure relates the pressures in the two phases. Since water is typically more strongly bound to rock than gas, 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.

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, 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. 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.

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 are required for calculations.

The relative permeability term for each phase is a modifier to the permeability which 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 conductivity, are rapidly emptied since the water is not so tightly bound 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, have suggested (e.g. /Pruess and Tsang 1990, Persoff and Pruess 1995, Mott and Rodwell 1998, Swift and Goodfield 2001/) that in the two-dimensional geometry of a fracture, the interactions between the two flowing phases, gas and water, restricts 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,

$$p_w = \rho_w g z + p_{w0} + p'_w \qquad (3\text{-}13)$$

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:

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

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 velocity relates to the volume flow of gas at the local pressure. For a given mass flow rate, which better represents the rate of production of gas from the wastes, 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 (this is not to say that it is easy for a continuous porous medium, but at least a starting point based on laboratory measurements is possible for rocks of a granular porous medium nature).

Secondly, there may be important features of the flow, particularly small-scale features, that are not captured by the two-phase flow model 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.

The two-phase flow situation that arises 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 the one 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 3-2 shows how gas flow is influenced by and influences geosphere variables and other processes. The handling in SR-Can is also indicated in the table and further described in Section 3.2.7.

Table 3-2. Direct dependencies between the process “Gas flow/dissolution” and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes. Affects viscosity.	Excavation/ operation/ resaturation	Gas flow neglected; no repository-induced gas and gas flow secondary relative to drawdown and water inflows to the repository.	Yes. But heat transport not significant through gas flow.	Excavation/ operation/ resaturation	Gas flow neglected; minor process, see Section 2.1 Heat transport.
		Temperate period	Properties at constant temperature.		Temperate period	Neglected; little significance, see Section 2.1 Heat transport.
		Permafrost Glaciation	Gas flow neglected; minor process.		Permafrost Glaciation	Gas flow neglected; minor process.
Groundwater flow	Yes. Groundwater flow and gas flow are coupled and flowing ground-water can transport dissolved gas, which may subsequently come out of solution.	Excavation/ operation/ resaturation	Gas flow neglected (see row Temperature above).	Yes. Groundwater flow and gas flow are coupled.	Excavation/ operation/ resaturation	Gas flow neglected; minor process, see Section 3.1 Groundwater flow.
		Temperate period	Considered in estimates of the capability of the geosphere to transport gas.		Temperate period	Effect of gas bubble flow on the water flow (by entrainment of water) is taken into account.
		Permafrost Glaciation	Neglected; minor process.		Permafrost Glaciation	Neglected; minor process.
Groundwater pressure	Yes. See row Groundwater flow above.	Excavation/ operation/ resaturation	Gas flow neglected (see row Temperature above).	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 period	See row Groundwater flow above.		Temperate period	See row Groundwater flow above.
		Permafrost Glaciation	Neglected; minor process.		Permafrost Glaciation	Neglected; minor process.
Gas flow						
Repository geometry	Yes. Affects the distribution of gas flow paths in the geosphere.	Excavation/ operation/ resaturation	Gas flow neglected (see row Temperature above).	No. Does not directly affect the geometry of deposition holes and tunnels.	–	–
		Temperate period	Deposition tunnel geometry considered in estimates of the capability of the geosphere to transport gas.			
		Permafrost Glaciation	Neglected; minor process.			
Fracture geometry	Yes. Geometrical configuration of fractures governs the gas flow.	Excavation/ operation/ resaturation	Gas flow neglected (see row Temperature above).	Yes. Gas pressure could induce rock fracturing.	Excavation/ operation/ resaturation	Gas flow neglected; minor process.
		Temperate period	Site-specific DFN model in estimates of the capability of the geosphere to transport gas.		Temperate period	Neglected; scoping calculations show that gas can be transported away from the repository without requiring a larger overpressure.
		Permafrost Glaciation	Neglected; minor process.		Permafrost Glaciation	Neglected; minor process.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 period	Neglected; see row Fracture geometry above.
					Permafrost Glaciation	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	No. But could be an insignificant coupling through gas composition as well as through groundwater flow (see Section 3.1).	–	–	Yes. Constituents transported in gas phase may dissolve in water.	All	Gas flow neglected; minor process (see also Section 5.10).
Gas composition	Yes. Gas composition affects gas phase flow properties (but insignificant).	Excavation/ operation/ resaturation	Gas flow neglected (see row Temperature above).	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 period	Neglected; main gas generated is hydrogen.		Temperate period	Neglected; main gas generated is hydrogen.
		Permafrost Glaciation	Neglected; minor process.		Permafrost Glaciation	Neglected; minor process.
Structural and stray materials	Yes Grouting can affect gas escape from the repository.	All	Neglected; grouting degradation expected to be fast.	No. Does not affect structures and materials	–	–
Saturation	Yes. Gas permeability depends on saturation through relative permeability.	Excavation/ operation/ resaturation	Gas flow neglected (see row Temperature above).	Yes. May alter saturation.	Excavation/ operation/ resaturation	Process neglected in calculations of inflow to tunnels.
		Temperate period	Considered in estimates of the capability of the geosphere to transport gas.		Temperate period	Not made explicit in scoping calculations of gas transport.
		Permafrost Glaciation	Neglected; minor process.		Permafrost Glaciation	Neglected; minor process.

3.2.3 Boundary conditions

The main boundary and initial conditions to be established are the gas production rate and the prevailing 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). The effect of 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 Stripa /Olsson 1992/, 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 to 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 capacity of the geosphere to transport gas needs to be assessed for site-specific conditions.

In a recent modelling study /Painter and Sun 2005/, it is shown 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. If the transient inflows and/or unsaturated zone dynamics are of interest, an unsaturated description of the flow will be needed. 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).

3.2.5 Time perspective

The timescale for gas transport from the repository to the atmosphere is expected to be much shorter than the timescale for water transport. On the other hand, the period over which gas may be generated from defective waste canisters is expected to be considerable (more than 250,000 years).

3.2.6 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.

3.2.7 Handling in the safety assessment SR-Can

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 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, 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 re-saturation are to be assessed. Therefore, gas-phase flow is not modelled for this phase of repository development within SR-Can.

Temperate period

The issue of main concern to be assessed is whether the capacity of the fractured geosphere is sufficient that gas generated in the repository (canisters) can be transported rapidly through the geosphere and up to the biosphere. Such rapid transport would ensure 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 there. 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. If such transport conditions prevail, the approach 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.

If it is unexpectedly found that significant quantities of gas could be trapped and stored in the repository environment, more detailed analyses of the impact of the gas phase on groundwater flow may be needed. Separate computational tools from those used for the groundwater flow simulations would then be applied.

Permafrost and glaciation

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-Can Climate report /SKB 2006e/.

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 would collect beneath the permafrost. It is not expected that this would significantly affect the groundwater flow, for example, compared to the effect of the permafrost itself. However, it could mean that any gas that had acculumated 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-Can.

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

Earthquakes

Not relevant.

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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 permability 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

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 is subject to uncertainty. 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-Can

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 predicted gas generation rate. These arguments are based on average values of fracture characteristics as determined from hydraulic tests and the calibration of groundwater flow models. Such factors as the width of a gas channel through fractures of the transmissivity that is required to support the required gas flow are considered as well as the velocity of bubbles through the fractures, and the extent to which components might be removed from the gas phase by dissolution in groundwater during migration. Although the elements of the flow characteristics considered will represent gross oversimplifications of actual gas flow channels through rough fractures with complex orientations and interconnections, the approach should be robust provided that 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. Should this not be the case, then consideration would need to be given to the possibility of developing more sophisticated approaches to assess gas migration from a repository, although such approaches would be faced with data acquisition difficulties.

Input data and data uncertainties in SR-Can

Assessment of gas migration behaviour requires an assessment of the likely, or an upper bound to this gas generation rate from defective waste 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 data extracted from this are reasonable.

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, which extends from the Kola Peninsula and Karelia through Finland and Sweden to southern Norway. The rock types that occur in different provinces of the Baltic Shield are approximately 900 to 2,500 million years old /SKB 2005ab/.

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/brittle material, of which the crust makes up the uppermost 45 km, resting on a viscoelastic mantle. Going into detail, the conditions in the Shield are complex. The thickness of the crust, for instance, varies significantly 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, looks 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 /Sundberg 1995/. The deformation of the Shield under load is further affected by the fact that it is crossed by a number of deformation zones that enable the different parts of the Shield to move relative to each other, for example the Protogine Zone, which constitutes the boundary of the Sveconorwegian province in the southwest.

The Baltic Shield is continuously subjected to a horizontal compression or "ridge push" due to seafloor spreading from the Mid-Atlantic Ridge at the western tectonic plate boundary /Muir Wood 1993/ as well as to the collision with the African plate /Hakami et al. 2002/. The compression is probably an important factor for the development of the state of stress currently prevailing in the Swedish bedrock (see above) where the maximum principal stress tends to be horizontal and oriented NW-SE, i.e. in the ridge-push direction. This is true in the southern and central parts of Sweden, whereas the picture is more fragmented in the northernmost parts of the country, where a possible tendency towards N-S orientation of the maximum principal stress can be observed /Juhlin et al. 1998/.

Theories positing that the mechanical equilibrium in the bedrock is determined by a balance between rock stresses and frictional forces in large fracture zones have been proposed and entail that the rock mass adapts continuously by means of friction-controlled displacements in the major fracture zones /Scholz 1990, Leijon 1993, Zoback and Townend 2001/.

Current tectonic conditions can be judged to have been constant for the past two million years, whereas the state of stress may have persisted for the most part during the past 25 million years /Muir Wood 1995/.

The Shield has also been subjected to loading due to glaciations and will probably be subjected to new such loads /Wallroth 1997/. 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/. There are, however, some uncertainties with regard to what state of stress will prevail under, and at the margin of, the ice cap, particularly with respect to the near surface shear stress, and what time scale applies to the recovery of the stress field.

To assess the state of stress under the ice sheet, the simplest approach is to assume that the vertical stresses increase by an amount that is equal to the ice load, and that the increase of the horizontal stresses can be calculated with simple expressions from elasticity theory, which gives a stress increase that is approximately one-third of the vertical stress increment. This model entails that the state of stress is less deviatoric and the rock, therefore, more stable with less tendency towards shear displacements /Muir Wood 1993/. This approach has been used in previous studies of the mechanical effects of a glacial cycle on a deep repository /Shen and Stephansson 1996/. Other models entail that the horizontal stresses will be influenced by the extent of the ice load, by the flexural stiffness of the crust and the uppermost part of the mantle, and by the rheological properties of the viscoelastic medium underneath the elastic plate. Such models give a more complex picture of the horizontal stresses in the upper parts of the crust /Peltier 1974, Wolf 1991, Lund 2005/, with increases in horizontal compressive stresses under the ice and reductions outside the ice margin. The issue is addressed in the SR-Can Climate report /SKB 2006e/.

The timescale for the downwarping of the crust during the growth of the ice sheet, as well as the timescale for land uplift after melting of the ice sheet, depends on the rheological properties of the viscoelastic material underneath the elastic/brittle plate. Land uplift following the most recent glaciation (glacial rebound) is still proceeding, at different rates in different parts of the Shield, which means that the bedrock is still being deformed. Of a vertical subsidence of approximately 900 m in the most depressed portion of the Shield, approximately 140 m is now estimated to remain /Kakkuri 1986/.

The current maximum land uplift rate is estimated to 9.0 mm/yr using a hundred years of sea- and lake-level data /Ekman 1996/ and to 10 mm/yr using seven years of continuous GPS data /Johansson et al. 2002/. The deformations that take place in conjunction with the continuing differential uplift result in horizontal strains of the crust in the Shield. Calculations show that these strains may be 10^{-9}/year /Muir Wood 1993/, which in one hundred years can give a relative displacement of 1 cm for points at a distance of 100 km from each other.

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

The question of strain rate magnitudes and strain rate distribution has been addressed within the BIFROST project /BIFROST 1996, Johansson et al. 2002/. The BIFROST project has analysed permanent GPS station data from Scandinavia since 1993. The large-scale, three-dimensional crustal motion in Scandinavia is currently determined to an accuracy of 0.3–0.4 mm/yr in the horizontal components and 1.3 mm/yr in the vertical component /Johansson et al. 2002/. The maximum recorded vertical rate is approximately 11 mm/yr and the maximum horizontal rate exceeds 2 mm/yr at several sites. Analysing the 3D velocity field in a Eurasia comoving reference frame, the data fit models of glacial isostatic adjustment (GIA) /Lambeck et al. 1998/ with residuals on the order of 1–2 mm/yr /Milnes et al. 2004/. There has been no analysis of the BIFROST strain rates as of yet.

The large-scale movements that take place in the Shield determine the boundary conditions for the long-term mechanical evolution of the repository's host rock. If no, or only little, adjustment, i.e. strain release, occurs by means of aseismic or seismic fault motion, stress changes in the Earth's crust and changes of the loads that act on the host rock will be obtained. A large-scale strain rate on the order of 10^{-9}/year would then give a horizontal stress change of up to about 5 MPa in one hundred thousand years. Large ice sheets might suppress strain release through fault motion, due to the added normal stress from the weight of the ice /Johnston 1987/. Strain would then accumulate under the ice sheet only to be released at the time of deglaciation, causing large earthquakes, such as 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. The magnitude of the earthquakes has rarely exceeded 5.0 in modern times /Slunga 1991/. The earthquakes in the Kattegatt in 1985 and in Skövde in 1986 were, for example, of magnitudes 4.6 and 4.5, respectively /Muir Wood 1993/. An earthquake occurs when strain energy that has accumulated over a long time of slow deformations is suddenly released by shear displacements along a major or minor 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 30 /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 150,000 times more energy is released than by typical modern Swedish bedrock earthquakes, for instance the magnitude 4.5 events in Skövde and Kattegatt.

It follows from the above that large events can only occur on very large discontinuities, because the seismic moment is directly proportional to the area of the displaced surface, and because the maximum possible average displacement cannot amount to more than a fraction of the fracture's extent in its own plane.

An earthquake can be perceived as a sudden local rupture at an asperity (roughness) that is loaded increasingly due to 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 displacement has become sufficient to cause rupture. The altered stress picture around the fracture zone may lead to new stress concentrations around other asperities, either in the fracture zone where the earthquake occurred or in a nearby zone. If enough strain energy has not been released to restore stability in the region, then 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 fracture zone in which the earthquake took place, and dynamic effects in the form of mechanical oscillations 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 during some earlier epoch 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. Deformations due to tectonic movements, “ridge push”.
2. Deformations due to the differential land uplift that is still in progress since the most recent ice age, “glacial rebound”.

Furthermore, there is evidence that intense seismic activity, postglacial faulting, took place in Lapland in direct conjunction with the melting of the most recent ice cap (on the Lansjärv Fault, the Parvie Fault, etc.). 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/. The magnitude of the Lansjärv earthquake is calculated to have been 7.8.

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. Deglaciation proceeded more rapidly in the area southeast of the remaining ice cap, whereas it proceeded much more slowly in the northwest. This led to a highly asymmetrical unloading where the two deglaciation zones approached one another. Furthermore, during the glaciation the area lay beneath the north-western flank of the ice cap, which means that the stress contribution from radial mantle movements was added to the pre-existing NW-SE oriented stresses. When the vertical load rapidly diminished, large shear stresses were created which triggered the earthquake.

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/. There is also agreement that the fault displacements took place as a reactivation of existing fracture zones rather than new fracturing.

For the safety analysis, 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/, the possibility that this may happen in the future 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 models /SKB 2005ab, 2006a/. 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 intact rock and the fractures are more important than corresponding 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 adopted 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 /SKB 2005ab, 2006a/.

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 microfracture 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. Elastic intact rock deformations create loads on fractures, possibly leading to reactivation and slip. Depending on the slip magnitude, there may be time-dependent growth of microcracks 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.

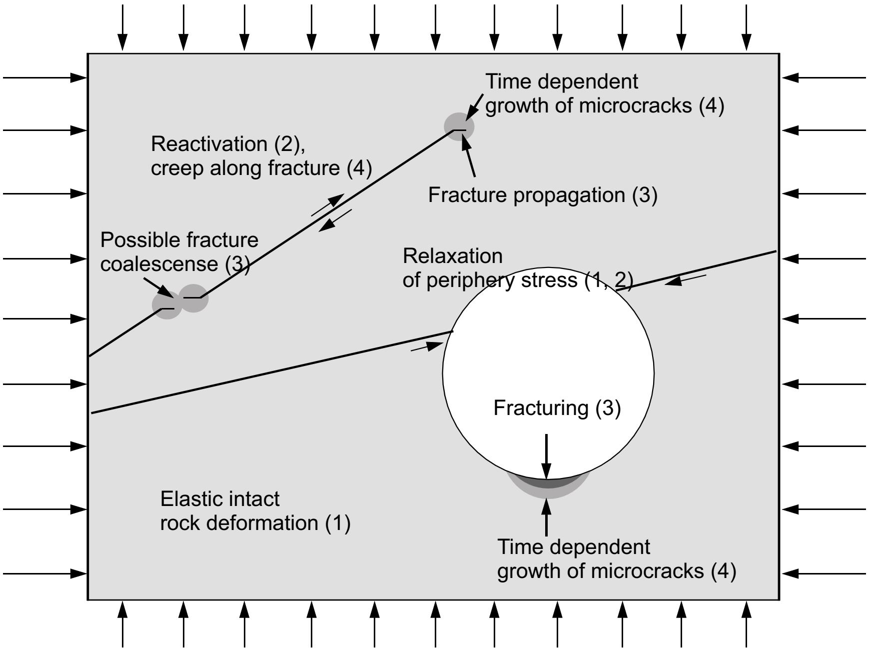

Figure 4-1. *Schematic showing examples of mechanical SR-Can geosphere processes in rock volume under load: Displacements in intact rock (1), Reactivation (2), Fracturing (3) and Creep displacements (4).*

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 microcracks at approximately 50% of the peak uniaxial strength. In the repository, these microcracks 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 of 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-Can is also indicated in the table and further described in Section 4.2.7.

Temperature; 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.

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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes. Determines thermal expansion.	Excavation/operation	Neglected; little significance compared with impact of stress.	No.	–	–
		Temperate	Thermal load conditioned to site specific layout.			
		Permafrost	Process not handled in SR-Can, see Section 4.2.7.			
		Glaciation	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.	–	–
Gas 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. Bentonite swelling pressure and pore pressure at walls of deposition holes.			
		Permafrost	Process not handled in SR-Can, see Section 4.2.7.			
		Glaciation	Stresses at repository depth from ice/crust/mantle model, see Climate report /SKB 2006e/. Otherwise same as for Temperate.			
Matrix minerals	Yes. Controls stress-strain relation.	Excavation/operation	Site-specific rock mechanics property data.	No.	–	–
		Temperate	Site-specific rock mechanics property data.			
		Permafrost	Process not handled in SR-Can, see Section 4.2.7.			
		Glaciation	Site-specific rock mechanics property data.			

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Fracture minerals	No.	–	–	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 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 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 /Follin and Hermanson 1997/. 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 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 sites under investigation, values of intact rock parameters are determined in the laboratory and reported in the site descriptive models, e.g. /SKB 2005ab, 2006a/. For parameters that are relevant to intact rock displacements, i.e. Young´s modulus, Poissons'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 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 has taken place. During the temperate period the regions of failure, as well as regions of time-dependent growth of microcracks, increase in volume because of the thermal load. However, for the walls of tunnels and deposition holes, the excavation has a larger impact on the stresses than following loads /Martin et al. 2001, Hökmark et al. 2006/, which means that that volume increase is modest. Brittle failure and microfracture growth are aspects of the fracturing process and the creep process, and are dealt with in the following sections.

4.2.6 Natural analogues/observations in nature

Not relevant.

4.2.7 Handling in the safety assessment SR-Can

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 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 failure around the repository openings and to obtain estimates of possible permeability changes caused by shear and normal fracture displacements.

Model; The 3DEC discrete fracture models described in /Hökmark et al. 2006/.

Boundary conditions; Zero normal stress 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 period

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 points of departure for the simulation of the temperate period with thermal load, development of buffer swelling pressure and pore pressure. Thermal loads are conditioned to site-specific layouts.

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 discrete fracture models described in /Hökmark et al. 2006/.

Boundary conditions; Zero normal stress assigned at the ground surface and zero or 10 MPa of swelling pressure at the deposition hole walls, depending on the swelling pressure assumption. The swelling pressure of the backfill, expected to be not more than a few hundred kPa, is ignored. Different assumptions are made regarding the pore pressure. If the pore pressure is assumed to be restored during the period, an additional 5 MPa boundary stress is specified at the walls of the openings.

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.

Permafrost

The process will be 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.

Glaciation

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 discrete fracture models described in /Hökmark et al. 2006/.

Boundary conditions; Normal stress assigned at the ground surface and horizontal stress at repository depth according to ice/crust/mantle model /Lund 2005/. Swelling pressure of 10 MPa plus 5 MPa of pore pressure assigned at the walls of the deposition hole. Swelling pressure of backfill, expected to be a few hundred kPa, 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-Can

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

Input data and data uncertainties in SR-Can

Parameter values of material properties used in the 3DEC models are based on the site descriptive models. These data are found in the SR-Can data report /SKB 2006d/.

4.3 Reactivation – displacement along existing discontinuities

4.3.1 Overview/general description

The most significant mechanical process in the geosphere from the 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 deviant mechanical properties. On the repository scale, however, it is appropriate 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 /Hökmark 1990, Barton et al. 1985/. 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 1990ab/.

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. Fracture zones, which have small normal stiffness, on the other hand, 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, elaborated 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's model for shear displacement and an ideal elastoplastic model with a Coulomb failure criterion.

/Barton and Vik 1988/ and /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 safety are controlled by strength parameters, i.e. by cohesion and friction.

For fracture zones, i.e. structures composed as systems of single fractures, the mechanical behaviour is more complex. Zone thickness and fracture frequency, plus degree and nature 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-Can is also indicated in the table and further described in Section 4.3.7.

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.

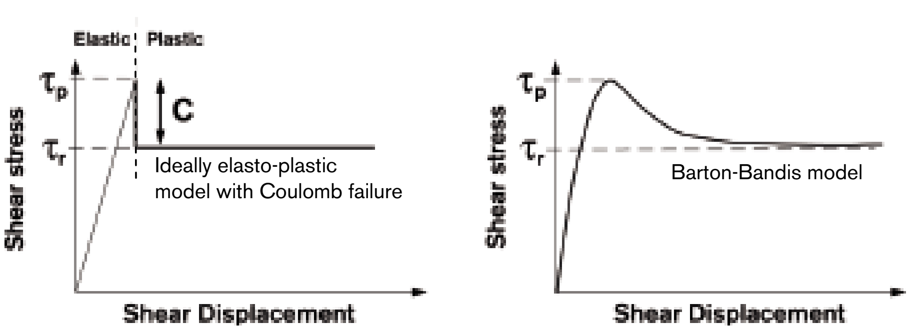

Figure 4-2. *Stress – deformation relations for single fracture. τ_p = strength at failure, τ_r = residual strength, c = cohesion.*

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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	No. But indirectly via stresses.	–	See Section 4.2.	No.	–.	–
Groundwater flow	No.	–	–	No. But indirectly through fracture geometry.	–	–
Groundwater pressure	Yes. Effective stress reduction has influence on shear strength.	Excavation/ operation	Included in the model as fracture pore pressure.	Yes. But only for rapid displacements.	All	Not considered.
		Temperate	Included in the model as fracture pore pressure.			
		Permafrost	Process not handled in SR-Can, see Section 4.3.7.			
		Glaciation	Included in the model as fracture pore pressure.			
Gas 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.	Excavation/ operation	Generic fracture systems.	Yes.	All	Aperture changes evaluated from fracture stress results.
		Temperate	Generic fracture systems.			
		Permafrost	Process not handled in SR-Can, see Section 4.3.7.			
		Glaciation	Generic fracture systems.			
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 calculated in model. Zero normal stress at ground surface. Bentonite swelling pressure and pore pressure at walls of deposition holes.			
		Permafrost	Process not handled in SR-Can, see Section 4.3.7.			
		Glaciation	Stresses at repository depth from ice/crust/ mantle model, see Climate report /SKB 2006e/. Otherwise same as for temperate period.			

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Matrix minerals	Yes. Affects mechanical properties of fracture surfaces.	Excavation/operation	Site-specific rock mechanics property data.	No.	–	–
		Temperate	Site-specific rock mechanics property data.			
		Permafrost	Process not handled in SR-Can, see Section 4.3.7.			
		Glaciation	Site-specific rock mechanics property data.			
Fracture minerals	Yes. Affects stress-deformation relations.	Excavation/operation	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.
		Temperate	Site-specific fracture property data.			
		Permafrost	Process not handled in SR-Can, see Section 4.3.7.			
		Glaciation	Site-specific fracture property data.			
Groundwater composition	No.	–	–	No.	–	–
Gas composition	No.	–	–	No.	–	–
Structural and stray materials	No	–	–	No.	–	–
Saturation	No	–	–	No.	–	–

Groundwater pressure; Pressure variations will give normal displacements, i.e. changes in mechanical aperture. In addition, there will be changes in fracture shear strength. 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 for water to move and pressures to keep approximately constant.

Gas 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 /Pollard and Segall 1987/ 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 maximal shear slip that can occur as a result of a shear stress increment. The analytical expression used here is based on a 2D solution valid for fractures with infinite extension in the out-of-plane direction. The 2D slip magnitudes were corrected by a factor of 0.7 to obtain the results for circular fractures shown in Figure 4-3 /Hakami and Olofsson 2002/.

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.

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 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 boundary normal stress, or boundary pressure, will vary due to effects of the glacial loading.

Earthquakes will generate additional static and dynamic loads.

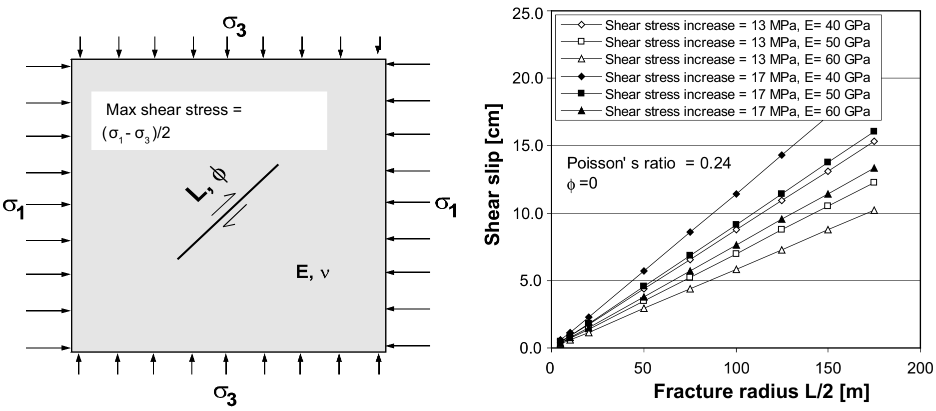

Figure 4-3. *Left: Schematics of fracture of extension L and with friction angle φ in elastic medium with Young's modulus E and Poisson's ratio ν. The maximum shear stress is found in planes at 45 degree angle to the major and minor principal stresses. Right: Shear displacement on a friction-free fracture following a shear stress increment as a function of fracture size for two load cases and for three assumptions regarding Young's modulus E.*

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). An overview is given by /Jing 2003/. 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

/Hökmark 1990/ and /Hökmark and Israelsson 1991/ simulated excavation of the Buffer Mass Test tunnel at Stripa with UDEC and 3DEC. The fractures were 10 to 20 m in length, with mechanical properties in accordance with laboratory determinations done on fracture specimens from the Stripa Mine /Barton and Vik 1988/. A material model similar to Barton's model was used in the UDEC study, whereas an ideal elastoplastic model with Coulomb's fracture criterion was used in the 3DEC study. Excavation of a half-scale deposition hole was also simulated in the 3DEC study. The calculated shear displacements amounted to 2–3 mm at most. /Johansson et al. 1991/ performed similar calculations with UDEC and 3DEC for a hypothetical repository in the Finnish bedrock, but assumed a larger strength in the fractures and furthermore analysed the thermomechanical effects of the deposited fuel. 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 version 1.2 site descriptive models /SKB 2005ab/, 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.

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.

/Israelsson 1996/ performed thermomechanical 3DEC calculations for a hypothetical repository in Äspö with nine, steeply-dipping, large fracture zones intersecting the hypothetical repository area. The maximum shear displacement was about 2 cm for pessimistic assumptions regarding the thermal power. Under these conditions, the aperture of the zones increased down to a maximum depth of about 200 m below the surface.

/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).

/Munier and Hökmark 2004/ conducted dynamic analyses of magnitude 6 earthquakes. The main objective was to find upper-bound estimates of secondary, or induced, shear displacement on repository host rock fractures. The study addressed fractures of 100 m radius and confirmed the validity of one of the assumptions made in /LaPointe et al. 1997/, i.e. that the static response overshadows the dynamic effects for small epicentre distances. Friction-free 100 m radius fractures were found to move less than 0.1 m at epicentre distances larger than 200 m. The study addressed earthquakes of magnitude 6, but the results are suggested to be valid also for larger earthquakes, provided that the stress drop associated with the fault displacement is in the same range as assumed in the calculations (15 MPa) or smaller.

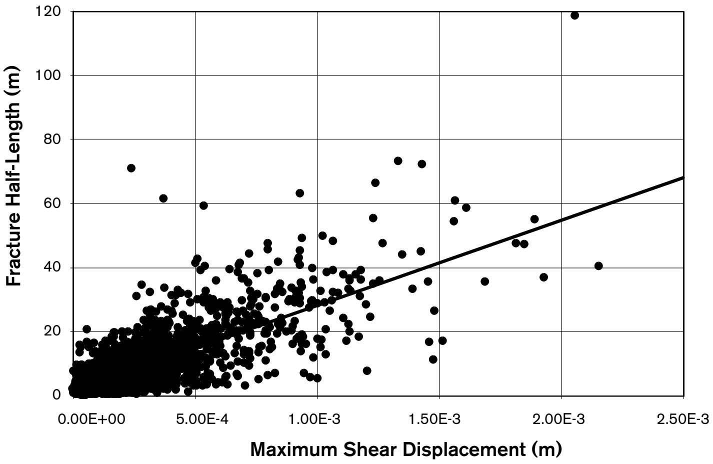

Figure 4-4. *Shear displacement of fractures in the repository caused by an earthquake of magnitude 6.1 at a distance of 2 km from the repository as a function of the length of the fractures. The scatter around the regression line is due to the distribution in distances of the individual fractures from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

/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 the 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/.

4.3.5 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 glaciation cycles. Large-scale tectonic strain, i.e. ridge push, will 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 only in connection with glaciations, i.e. similar to the way postglacial faulting took place in northern Sweden after the last glaciation.

4.3.6 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.

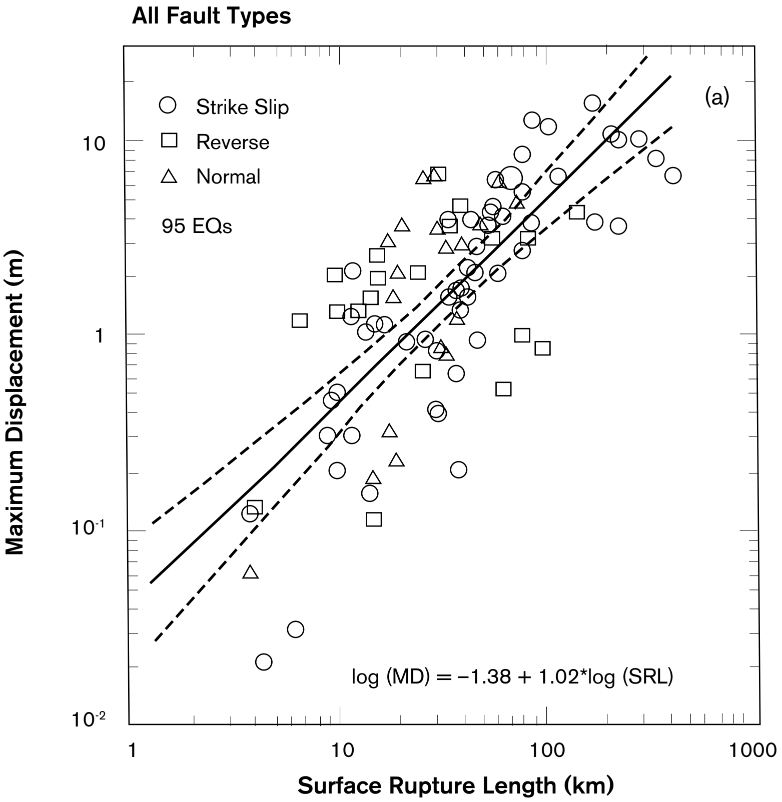

Figure 4-5. *Empirical relation between maximum displacement and observable length of fault structure that has been active in conjunction with an earthquake. The database consists of 95 earthquakes (from /La Pointe et al. 1997/).*

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 in 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 recording 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 where these displacements have taken place.

4.3.7 Handling in the safety assessment SR-Can

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/.

Boundary conditions; Zero normal stress assigned at 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 must be evaluated from fracture stress results. 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 0.1 m. According to regression relations given in /Wells and Coppersmith 1994/ a slip of 0.1 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 extraction ratio 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-Can.

Temperate period

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/.

Boundary conditions; Zero normal stress assigned at the ground surface and zero or 10 MPa of swelling pressure at the deposition hole walls, depending on the swelling pressure assumption. The swelling pressure of the backfill, expected to be not more than a few hundred kPa, is ignored. Different assumptions are made regarding the pore pressure. If the pore pressure is assumed to be restored during the period, an additional 5 MPa boundary stress is specified at the walls of the openings.

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 must be evaluated from fracture stress results. Effects on the groundwater pressure are not considered. Effects on fracture minerals (possibly increased amounts) are not considered.

Permafrost

The process will be 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.

Glaciation

The process is modelled in 3DEC studies of ice-load effects, using stresses obtained from ice/crust/mantle models /Lund 2005/ 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 estimated from results of hydromechanical simulations performed within the DECOVALEX project. The probability of earthquakes of magnitude ≥ 6 occurring within 5 km radius from the site centres 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/. For earthquake consequences, see below.

Boundary conditions; Normal stress assigned at the ground surface and horizontal stress at repository depth according to the ice/crust/mantle model /Lund 2005/. Swelling pressure of 10 MPa plus 5 MPa of pore pressure assigned at the walls of the deposition holes and 5 MPa of pore pressure at the tunnel walls. Swelling pressure of backfill, expected to be a few hundred kPa, ignored.

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 must be evaluated from fracture stress results. Effects on the groundwater pressure are not considered. Effects on fracture minerals (possibly increased amounts) are not considered.

Earthquakes

An analytic method for estimating the probability of canister/fracture intersections /Hedin 2005/ is used to calculate the fraction of canisters that could be damaged if all host rock fractures were to slip maximally, i.e. according to upper bound estimates of secondary, earthquake-induced displacements. Preliminary, pessimistic upper bound slip estimates are given by /Munier and Hökmark 2004/ and more recent and realistic ones by /Fälth and Hökmark 2006/. The critical fracture radius, i.e. the minimum radius of fractures that could slip sufficiently (0.1 m) to damage a canister, is determined from the estimates given in /Fälth and Hökmark 2006/. For fractures located with their centre at distances of 100–200 m from potential earthquake faults the critical radius is 75 m. At distances larger than 200 m the critical radius is 150 m.

Site-specific Discrete Fracture Network models, i.e. statistical models that describe fracture densities and size-frequency relations, are used as input to the analytical canister/fracture intersection calculations. The canisters are assumed to be deposited blindly according to the design rules, i.e. the canister spacing rules /SKB 2004a/ and the respect distance rules /Munier and Hökmark 2004/, without regard to possible intersections of discriminating fractures (radius > 150 m). The fraction of damaged canisters is calculated assuming one of the zones that have been assigned a seismic respect distance to be a potential earthquake fault. The zone with the largest number of canisters at distances between 100 m and 200 m will be selected for this. For the majority of the canisters the critical radius will be 150 m and for those within the 100–200 m band close to the selected zone, it will be 75 m.

The calculated canister damage fraction considers that all fractures will reactivate and all fractures will host their maximum possible slip. Additional assumptions are that the fracture intersects the canister in the most unfavourable position and angle, and that the canisters are deposited blindly. The risk is actually very much smaller and is assessed by estimating the following:

- The probability that a discriminating fracture will remain undetected after tunnel mapping.
- The probability of seismic events in the immediate vicinity of the repository.
- The induced displacements. On average, fractures will displace less than their maximum theoretical value, due to unfavourable orientations for reactivation to occur and interaction with nearby fractures.

Model; Analytical model described in /Hedin 2005/.

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

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.

For secondary slip displacements induced by earthquakes, there is some uncertainty regarding the relative importance of stress drop and moment magnitude for large events. The theory of stress drop being independent of magnitude was proposed by /Scholz 1990/ and used by /Fälth and Hökmark 2006/ for estimating secondary effects of seismic events that are too large to simulate dynamically with present-day computational capabilities. In the numerical analyses of magnitude 6 earthquakes, the dynamic effects turned out to be relatively small compared to the static effects. There is some uncertainty whether this holds true equally well for larger earthquakes.

Model simplification uncertainties in SR-Can

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.

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 and Hökmark 2006/, i.e. the calculated secondary displacements were not influenced by frictional or viscous damping. This may mean that secondary displacements were overestimated.

The earthquake source mechanism was idealised with a 15 MPa average of stress drop regularly distributed over the rupture area, whereas the pattern of stress drop distribution may be complex and irregular for real earthquakes. Typically, the stress drop will be smaller than the average on the majority of the rupture area (see for instance /Sekiguchi et al. 2004/) with the maximum stress drop occurring at large depths, far below the repository horizon. The effects of this simplification are difficult to quantify, but are likely to mean overestimated secondary displacement bounds.

Input data and data uncertainties in SR-Can

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-Can Data report /SKB 2006d/.

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, a value relevant of intact rock rather than of rock masses, which typically have mean values of about 60 MPa with considerable variability /SKB 2005ab/. If a lower rock mass value, for instance 60 GPa, had been assumed in the earthquake analyses, then the calculated secondary displacements would have been correspondingly larger. However, the lower value of rock mass modulus is largely due to the aggregate effect of many fractures that slip by different amounts, meaning that the use of a high modulus of elasticity is consistent with the pessimistic approach of disregarding the frictional damping effects of slipping fractures.

There is an uncertainty regarding the validity of the stress drop figure, 15 MPa, for the type of earthquakes considered in the safety analysis, i.e. postglacial fault displacements. However, the shear loads transferred to potential faults during a glaciation are probably smaller than the 15 MPa stress drop assumed in the dynamic analyses, at least in the upper part of the crust, which means that this particular uncertainty is pessimistically handled.

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 exceeds 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 4-3 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Can is also indicated in the table and further described in Section 4.4.7.

Table 4-3. Direct dependencies between the process “Fracturing” and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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.	Excavation/operation	Included in the model as fracture pore pressure.	No	–	–
		Temperate	Included in the model as fracture pore pressure.			
		Permafrost	Process not handled in SR-Can, see Section 4.4.7.			
		Glaciation	Included in the model as fracture pore pressure.			
Gas flow	No.	–	–	No. But indirectly through changes in fracture geometry.	–	–
Repository geometry	No. But indirectly through stresses.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Fracture geometry	No. But indirectly through stresses.	Excavation/ operation	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. Assessment of EDZ based on experience and observations from blasting of TASQ tunnel in Äspö HRL.
		Temperate	See Section 4.3.		Temperate	Scope and extent of fracturing in near-field rock evaluated from stress results and observations from the APSE experiment.
		Permafrost	Process not handled in SR-Can, see Section 4.4.7.		Permafrost	Process not handled in SR-Can.
		Glaciation	See Section 4.3.		Glaciation	Evaluated from stress results, including risk for hydraulic fracturing.
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 calculated in model. Zero normal stress at ground surface. Bentonite swelling pressure and pore pressure at walls of deposition holes.			
		Permafrost	Process not handled in SR-Can, see Section 4.4.7.			
		Glaciation	Stresses at repository depth from ice/crust/ mantle model, see Climate report /SKB 2006e/. Otherwise same as for temperate period.			
Matrix minerals	Yes. Affects mechanical properties of fracture surfaces.	Excavation/ operation	Site-specific rock mechanics property data.	No.	–	–
		Temperate	Site-specific rock mechanics property data.			
		Permafrost	Process not handled in SR-Can, see Section 4.4.7.			
		Glaciation	Site-specific rock mechanics property data.			
Fracture minerals	No.			Yes. Fracturing can create new fracture surfaces with different mineralogy.	All.	Not considered in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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; 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 analyses. 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 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; Fracturing can expose new fracture surfaces with different mineralogy.

Saturation; Differences in strength properties between saturated and unsaturated samples of rock exist. These small differences are neglected.

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 Chunlin 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.

/Johansson and Hakala 1995/ studied the state of excavation-induced stress around the intersection of a tunnel and a deposition hole for different assumptions concerning the local primary rock stresses. The study was done numerically with a 3D continuum code, assuming the rock to be linearly elastic. The area around the deposition hole was then divided into categories with respect to how the state of stress was related to the different stages in the evolution of brittle failures that had been identified at the URL in Canada /Martin 1994/. The results showed that for primary stresses roughly corresponding to conditions at 1,000 m depth, only insignificant areas were in direct failure states, whereas slightly larger areas (maximum depth approximately 150 mm from deposition hole wall) were in a state of unstable fracture growth, i.e. with the possibility of spalling. A slightly larger area (to a maximum depth of approximately 400 mm) still was in a state where fracturing had been initiated (stable fracture growth). At stresses corresponding to a depth of 500 m, stress levels corresponding to direct failure or unstable fracture growth were not obtained anywhere. In all analyses, the least favourable tunnel orientation was assumed, i.e. with the tunnel axis perpendicular to the largest primary principal stress.

/Hökmark 1996/ performed thermomechanical elastic 3D calculations of the state of stress around deposition holes. The analysis showed that the areas that were in a potential failure state after heating were restricted to small volumes at the intersection of tunnel and deposition hole and to even smaller areas along the sides of the boreholes. The maximum depth of potential failure from the wall of the deposition hole was about 300 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 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. Vertical rod-shaped heaters were installed close to the side of the slender pillar. The tangential stress in the pillar could be 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. The geometry of the failed zone was similar to the one 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.

4.4.5 Time perspective

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

4.4.6 Natural analogues/observations in nature

Not relevant.

4.4.7 Handling in the safety assessment SR-Can

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. Assessment of the EDZ is made using experience and observations made during blasting of the TASQ tunnel in Äspö HRL /Olsson et al. 2004/.

Model; The 3DEC model described in /Hökmark et al. 2006/.

Boundary conditions; Zero normal stress assigned at 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 determines the values of property parameters and is included indirectly.

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

The excavation activities may, in theory, 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-Can.

Temperate period

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. 2006/.

Boundary conditions; Zero normal stress assigned at the ground surface and zero or 10 MPa of swelling pressure at the deposition hole walls, depending on the swelling pressure assumption. The swelling pressure of the backfill is ignored (see general boundary condition statement above). Different assumptions are made regarding the pore pressure. If the pore pressure is assumed to be restored during the period, an additional 5 MPa boundary stress is specified at the walls of the openings.

Handling of variables influencing the process; Groundwater pressure, fracture geometry and rock stresses are included in the model. 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 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 in the rock/buffer interface (cf. gas flow/dissolution process, Section 3.2).

Permafrost

The process will be 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. Possible fracturing due to freezing of the tunnel backfill will be handled in SR-Site.

Glaciation

Estimates of the scope and extent of fracturing in the near field are made using results obtained from 3DEC near-field models. The risk for hydraulic fracturing because of high pore pressures is assessed using results of ABAQUS hydromechanical glaciation model. Fracturing due to freezing of the tunnel backfill will be handled in SR-Site.

Model; The 3DEC model described in /Hökmark et al. 2006/.

Boundary conditions; Normal stress assigned at the ground surface and horizontal stress at repository depth according to ice/crust/mantle model /Lund 2005/. Swelling pressure of 10 MPa plus 5 MPa of pore pressure assigned at the walls of the deposition holes and 5 MPa of pore pressure at the tunnel walls. Swelling pressure of backfill, expected to be a few hundred kPa, ignored.

Handling of variables influencing the process; Groundwater pressure, fracture geometry and rock stresses are included in the model. In addition, 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

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 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-Can, the nuances of the process are not essential.

Model simplification uncertainties in SR-Can

The hydraulic properties of the EDZ are not assessed by means of numerical modelling. The EDZ hydraulic models will be 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 exceeded.

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. 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-Can

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-Can Data report /SKB 2006d/. Empirical data are obtained from the APSE experiment. These data are also given in the SR-Can Data report /SKB 2006d/.

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 1993/. Extrapolating strain rates, recorded during constant load tests, suggests accumulated total strains of between 0.1% and 0.3% after about 1 million years /Glamheden and Hökmark 2006/, meaning that creep in intact rock is not a concern for the deep repository. In jointed rock masses of crystalline rock, all significant creep can be approximated to occur along fractures and fracture zones /Glamheden and Hökmark 2006/.

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. 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 about 10% for filled fractures /Glamheden and Hökmark 2006/.

The mechanisms controlling the creep process in fractures are described in /Pusch and Hökmark 1993/ and /Glamheden and Hökmark 2006/. 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.

4.5.2 Dependencies between process and geosphere variables

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

Temperature; Creep displacements may be promoted by high temperatures. For the bounding type estimates made in SR-Can, 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 not different from 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, but the effects are small and cannot be separated from direct effects of other stress changes.

Table 4-4. Direct dependencies between the process “Creep” and the defined geosphere variables and a short note on handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes.	All.	Process neglected; covered by construction-induced reactivation.	No.	–	–
Groundwater flow	No.	–	–	No. But indirectly through changes in fracture geometry.	–	–
Groundwater pressure	Yes. Affects fracture strength.	All.	Process neglected; covered by construction-induced reactivation.	No	–	–
Gas flow	No.	–	–	No.	–	–
Repository geometry	No. But indirectly through stresses.	–	–	No.	–	–
Fracture geometry	Yes.	All.	Process neglected; covered by construction-induced reactivation.	Yes.	All.	Process neglected; effect is small and cannot be separated from direct effects of other stress changes.
Rock stresses	Yes. Deviatoric stress state is necessary for the process.	All.	Process neglected; covered by construction-induced reactivation.	Yes.	All.	Process neglected.
Matrix minerals	Yes. Strength of asperities has impact on fracture properties.	All.	Process neglected; covered by construction-induced reactivation.	No.	–	–
Fracture minerals	Yes. Mineral-filled fractures will probably exhibit more creep than clean fractures.	All.	Process neglected; covered by construction-induced reactivation.	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.	–	–

Rock stresses; Creep deformations relax deviatoric stresses. Extensive creep deformations will tend to transform anisotropic stress states into more isotropic ones.

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 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 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 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 1993/.

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 1993/. /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. /Pusch 1996/ estimated the possible time-dependent deformation of deposition holes by assuming that the creep properties of the rock can be represented as a modulus of elasticity that decreases logarithmically with time. The estimate gave a maximum diameter decrease of 12 mm after 10,000 years.

/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 2006/. 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 a convergence of a deposition hole of less than 1 mm.

4.5.5 Time perspective

The process will by definition take place during all phases.

4.5.6 Natural analogues/observations in nature

No evidence relevant to the mechanical behaviour of crystalline repository host rock has been found.

4.5.7 Handling in the safety assessment SR-Can

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 period

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.

The assessment of the number of damaged canisters for the zero fracture shear stress approximation would depend solely on how many deposition holes are intersected by fractures of sufficiently great extension for the maximum shear deformation to exceed 0.1 m if they were friction-free. For reasonable load cases and for realistic values of the rock deformation parameters, this means fractures of at least 200 m in diameter, cf Figure 4-3. However, all relevant observations found in the literature show that creep, if it at all takes place, requires a minimum threshold shear stress corresponding to a substantial fraction of the laboratory-determined shear strength. Even if the strength, hypothetically, drops to that threshold uniformly over the entire fracture area, fractures would have to be larger than 300 m to slip by 0.1 m or more for reasonable load cases.

Intact rock creep requires stresses that will be found only in small volumes around the walls of the openings /Hökmark 2003/. The convergence of deposition holes found in all attempts to replicate the effects of the process in numerical models is insignificant.

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

Permafrost and glaciation

The process is neglected for the same reasons as for the temperate period. During the glaciation cycle, stresses will be higher /Hökmark et al. 2006, Lund 2005/, but not sufficiently high to change the outcome of the estimates.

Earthquakes

Not applicable.

4.5.8 Uncertainties

Uncertainties in mechanistic understanding

When it comes to the understanding of the rheological aspects of creep in crystalline rock masses and along fractures in crystalline rocks, the uncertainty is great, in particular for large time ranges, because there is no evidence for the existence of the phenomenon. The handling described above is based on upper-bound estimates of the effects of creep, rather than on descriptions of the mechanism. The uncertainty in mechanistic understanding is, therefore, without importance to the handling.

Model simplification uncertainties in SR-Can

The simplification of the creep problem, i.e. to neglect intact rock creep altogether and to use upper bound estimates of shear displacements of low-strength fractures to approximate effects of creep along fractures, is without uncertainties.

Input data and data uncertainties in SR-Can

No data are used in SR-Can.

4.6 Surface weathering and erosion

4.6.1 Overview/general description

The downwearing of the Earth's surface by exogenic processes is accomplished by weathering, erosion, and transportation of material. The combined effect of all weathering and erosion processes is referred to as denudation, i.e. denudation is the sum of the processes that results in the wearing away or the progressive lowering of continental relief.

Weathering

Weathering can be defined as structural and/or mineralogical break down of rock through the cumulative effects of physical, chemical and biological processes operating at or near the surface /Whalley and Warke 2005/. Weathering occurs when minerals are exposed to conditions at the surface that differ significantly from the conditions in which the minerals were formed. Rock approaches the surface through tectonic uplift or erosion of the overburden. In this context, the surface is defined as locations where the atmosphere, hydrosphere and biosphere interact with the lithosphere. The rate of weathering depends both on environmental conditions and mineralogical characteristics. The transformation of rock to soil by weathering is a prerequisite for the widespread development of flora and fauna on land.

When rock material come close to the surface, changes in pressure and temperature, and contact with surface water and biota, mean that it is no longer in a state of equilibrium, which in turn induces weathering. Weathering can, as mentioned above, be divided into physical, chemical and biological components. Physical or mechanical weathering occurs when volumetric expansion and related alteration of stresses break down the rock. Volume changes due to decreased overburden and stresses can result in the creation of fractures at various scales. Creation and volumetric alteration of salt crystals, freezing of water and freeze-thaw effects as well as thermal fatigue due to repeated (diurnal) heating and cooling, and thermal shock associated with fires, may also cause physical weathering. Chemical weathering comprises reactions between rock minerals and water. Examples are solution of minerals, carbonation, hydrolysis, hydration, and oxidation and reduction. Common to chemical weathering processes is that they depend on water composition, for example pH, salinity, CO_2 and redox potential. The prevailing temperature is another important parameter determining the type and efficiency of chemical weathering. Biological weathering comprises biochemical alterations of rock minerals and mechanical impact caused by drying of lichen and fungus, boring into rock by biota and root penetration into fractures and joints.

Erosion

Erosion can be defined as the removal and transport of bedrock and earth materials by a moving natural agent, such as air, water or ice. Erosion is often preceded by weathering and followed by sedimentation. Air or water flowing over a bed of loose particles generates a shear stress that tends to initiate particle movement /Collinson 2005a/. There is a critical boundary shear stress related to wind velocity and turbulence and water flow velocity above which particle movement occurs. With the exception of small grain sizes the critical shear stress will increase as the grain size increases. For small grain sizes (less than 0.1 mm, silt and clay) increased cohesive strength and lower surface roughness means that higher velocities are required to initiate movement.

The material is transported in two distinct ways, it is either carried along with the fluid or in intermittent contact with the bed /Collinson 2005b/. In the first case, fine-grained particles are supported by the upwards component of turbulence and carried away with the fluid in suspension. In the second case, generally referred to as bedload transport, coarser-grained material rolls (creep or reptation) or bounces (saltation) on the bed. Particles carried in suspension will enhance the erosive capability of the fluid by abrasion and particles moved by saltation, creep or reptation will set other grains in motion.

Wind erosion

Erosion and deposition of sediments by the wind, i.e. aeolian processes, occur in environments with sparse or non-existent vegetation, a supply of fine-grained sediments and strong winds, for example beaches, semi-arid or arid regions, periglacial regions, and agricultural fields /Lancaster 2005/. Aeolian processes depend on weathering or other natural agents, e.g. rivers and waves, to supply sediments for transport. Particle movement is achieved due to wind shear stress and atmospheric turbulence. Particles begin to move when wind forces exceed the effect of weight and cohesion; the first particles to move dislodge or impact other grains and the number of particles in movement increase exponentially. However, the particles reduce the near-bed velocity of the wind and the transport reaches a dynamic equilibrium state in a few seconds. The mass flux of particles is related to the wind shear velocity, abrasion and the impact of particles moved by saltation and creep. The latter mobilise fine grained material affected by cohesion but easily carried by the wind. Thus, the transport rate is limited both by wind shear velocity and supply of particles.

Fluvial erosion

Erosion and deposition of particles by water, i.e. fluvial erosion and deposition, is related to flow velocity. To generate water flow, a water supply and a flow gradient are required. Therefore, erosion by water generally requires a slope. However, erosion by water can also occur on bare surfaces as raindrops hit the surface and splash particles away. Fluvial erosion occurs on slopes, in ditches, brooks and rivers, and on beaches by wave action. Similar to wind erosion, erosion by water depends on shear stress and turbulence, and particles begin to move when water fluid forces exceed the effects of weight and cohesion. The relation between grain size, flow velocity and different modes of erosion and deposition are illustrated in a Hjulström-Sundborg diagram, see Figure 4-6.

Erosion on slopes provides material that is transported to brooks and rivers, and into lakes and the sea. When freshwater reaches the sea, particles can coagulate into larger flocks and sedimentation is accelerated. Erosion by water on a slope increases with increased intensity of rain or snowmelt, increased inclination and length of the slope and decreased resistance to erosion of the soil. As for wind erosion, the presence of vegetation reduces erosion rates.

Erosion on slopes can also be the result of mud flows, landslides, creep processes and avalanches. These processes result from the movement of masses of snow, earth and debris down a slope under the influence of gravity and can occur at scales from a few metres to several kilometres and at rates from metres per year to metres per second /Burns 2005/. The material can move by creep, sliding, flowing and falling. The movement of material is generally triggered by increased water content (for example from snowmelt), but earthquakes and volcanic eruptions can also cause material to move down a slope.

Glacial erosion

Glacial erosion is complex and depends on material properties of ice and rocks, ice thermodynamics, friction and lubrication, chemical effects and sub-glacial hydrology. In recent years, field interpretations of geomorphological features /e.g. Kleman et al. 1997/ measurements of cosmogenic radionuclides /e.g. Stroeven et al. 2002/ and ice sheet modelling /e.g. Näslund et al. 2003/ have resulted in a composite view on Fennoscandian glacial erosion. In some areas, dominated by basal frozen conditions, erosion has been limited, whereas in others, where basal melting and sliding have occurred, erosion may have been considerable.

Glacial erosion arises through several mechanisms – loosening of rock fragments, including fracturing and crushing, evacuation of fragments from the bedrock and their entrainment and transport in the ice /e.g. Sugden and John 1976, Drewry 1986/. There are two main processes of glacial erosion: plucking and abrasion. In addition, sub-glacial water can accomplish fluvial erosion. Plucking, or quarrying, can be described as the dislodgement of larger rock particles and blocks from the bedrock. Abrasion, or grinding of fine-grained material, occurs as ice carrying debris act on the bedrock surface. Water flowing in subglacial channels between the ice and the bed erodes the surface in the same way as water on an ice-free bed. Also, stresses caused by the ice load in combination with high water pressures, freeze-thaw effects and hydrofracturing result in fracturing and breakdown of the bedrock.

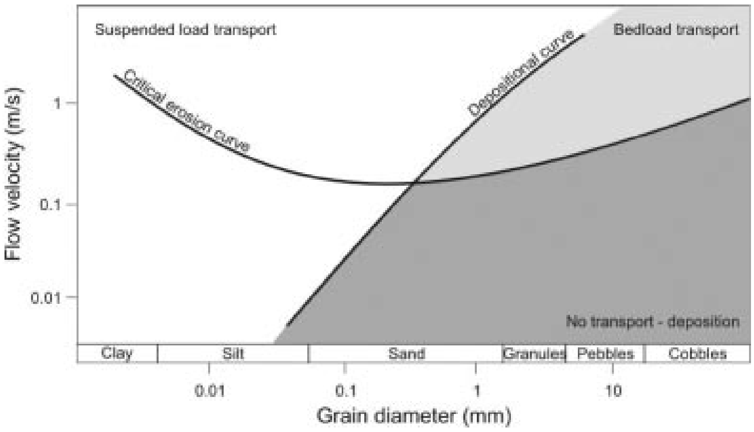

Figure 4-6. A Hjulström-Sundborg diagram showing the relation between flow velocity, grain size and erosion.

The current Fennoscandian landscape and landforms are the result of tectonic processes, weathering, erosion and sedimentation. As weathering, erosion and sedimentation all depend on environmental conditions, and also leave traces, the geomorphological record can give information on past environments. Glacial erosion is usually regarded as the main erosion process in Fennoscandia during the Quaternary. However, as great parts of Fennoscandia were not covered by ice during long periods of the Quaternary /Porter 1989/, other erosion agencies must also be considered /Lidmar-Bergström 1996, Lidmar-Bergström et al. 1997, Påsse 2004/.

4.6.2 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-Can is also indicated in the table and further described in Section 4.6.7.

Temperature affects chemical, physical and biological weathering.

Groundwater flow is not directly influenced by surface weathering and erosion. Surface weathering, erosion and redistribution of bedrock and sediments may influence groundwater recharge and indirectly alter the topography and thus flow gradients, however this impact is considered negligible.

Groundwater pressure is not directly influenced by surface weathering and erosion. Via altered topography, surface erosion may indirectly affect groundwater pressure. This impact is considered negligible.

Gas flow is not directly influenced by surface weathering and erosion. An insignificant indirect impact on gas flow may exist via altered topography and resulting changes in groundwater flow and pressure.

Repository geometry is not affected by surface weathering and erosion. Alteration of rock stresses as the result of erosion of bedrock and sediments is considered to be too small to affect repository geometry.

Fracture geometry close to the surface is affected, but at only a few metres depth bedrock is not directly influenced by surface weathering and erosion.

Prevailing **rock stresses** close to the surface affect the resistance to rupture and thus the loosening of rock fragments by air, water and ice. Surface weathering and erosion will breakdown, remove and redistribute rock and sediment masses and thus alter the load on the underlying bedrock. During the assessment period of up to one million years, the weathering and erosion depth is expected to be in the order of metres. Weathering followed by erosion removes rock and sediments, but the resulting decrease of vertical rock stresses is considered to be negligible at some tens to hundreds of metres depth.

The composition of **matrix minerals** affects their susceptibility to chemical and biological weathering and is also a factor determining the strength of the rock mass and hence its resistance to physical weathering and erosion processes. Rock minerals are altered by weathering. Only minerals close to the surface are affected by surface weathering and erosion.

Fracture minerals affect, and are affected by, surface weathering and erosion in the same way as matrix minerals. Further, the fracture minerals may affect the strength of the fracture and thus govern the loosening of rock material by water and ice. Only minerals close to the surface are affected.

Table 4-5. Direct dependencies between the process “Surface weathering and erosion” and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes.	All.	Process neglected; low erosion rates.	No.	–	–
Groundwater flow	No.	–	–	No. Process refers to weathering and erosion at the surface. Even if there is no absolute boundary between surface and groundwater this process only includes the action of surface water.	–	
Groundwater pressure	No.	–	–	No. See row Groundwater flow above.	–	–
Gas flow	No.	–	–	No. See row Groundwater flow.	–	–
Repository geometry	No.	–	–	No.	–	–
Fracture geometry	Yes. But only fractures close to the surface are relevant.	All.	Process neglected; low erosion rates (see also Section 4.7)	Yes. But only fractures close to the surface are relevant.	All.	Process neglected; low erosion rates, see also Section 4.7.
Rock stresses	Yes. Fracturing and loosening of rock material.	All.	Process neglected; low erosion rates.	No. But indirectly by the removal of rock and sediments.	–	–
Matrix minerals	Yes. Determines strength of rock mass and susceptibility to chemical and biological weathering.	All.	Process neglected; low erosion rates.	Yes. Affects matrix minerals close to the surface.	All.	Process neglected; low erosion rates, see also Section 4.7.
Fracture minerals	Yes. Affects strength of fractures and susceptibility to chemical and biological weathering.	All.	Process neglected; low erosion rates.	Yes. Affects fracture minerals close to the surface.	All.	Process neglected; low erosion rates, see also Section 4.7.
Groundwater composition	No.	–	–	Yes. Surface weathering may affect the composition of infiltrating surface water.	All.	Process neglected; low erosion rates
Gas composition	No.	–	–	No. But indirectly through groundwater composition	–	–
Structural and stray materials	No.	–	–	No.	–	–
Saturation	Yes. Affect resistance to weathering.	All.	Process neglected; low erosion rates.	No.	–	–

Groundwater composition affects weathering, erosion and sedimentation in fractures, but surface weathering and erosion is by definition only affected by the composition of surface water. However, the composition of surface water forming groundwater is affected by the surface environmental conditions including the properties of the soil layer. The soil layer is a result of surface weathering, erosion and sedimentation. Surface weathering may directly affect the composition of surface water forming groundwater; erosion may indirectly, by altering the soil layer, affect groundwater composition.

Gas composition does not directly affect weathering, erosion and sedimentation. Chemical weathering is the result of interactions between water and minerals. Surface weathering will alter the composition of the water forming groundwater. Both the gas content and the composition of the gas may be affected, but the impact of weathering on gas composition is indirect via groundwater composition.

Structural and stray materials are left in the bedrock and are not affected by surface weathering and erosion unless they are brought to the surface. With the limited amount of weathering projected, this should not occur.

The **saturation** of the rock mass and sediments affect their resistance to weathering. Even though minerals can bind water during chemical weathering, the saturation is not directly influenced by the degree or rate of surface weathering and erosion. However, altered mineralogy and porosity as a result of weathering and erosion may affect the saturation.

4.6.3 Boundary conditions

Weathering and erosion are complex processes affected by the prevailing environmental conditions. Given the characteristics of the rock, the degree of weathering depends on the availability of weathering agents such as salt, moisture, biota (e.g. microorganisms and lichens), and on the microclimatic conditions to which the rock is exposed. Weathering occurs in all climates, but high temperatures and humid conditions increase weathering rates. In areas where frost and/or permafrost occur, freezing and freeze-thaw effects are important geomorphic processes. However, weathering in periglacial environments is also affected by salt (in combination with freezing), wetting and drying, thermal fatigue and biological agents /French 1996/.

During temperate conditions, the dominant process is fluvial erosion. During permafrost conditions, when the climate can be expected to be dryer and vegetation sparse, wind erosion may also be important. During spring when the snow melts, there may be significant erosion of sediments in the active layer in periglacial permafrost areas. During glacial conditions, the erosion is mainly affected by the basal conditions of the ice sheet. In areas where the ice is frozen to the bed, the ice acts to preserve its subsurface and practically no erosion occurs, whereas in areas of basal melting erosion of bedrock and pre-existing sediment is likely to occur, with more erosion generally associated with faster ice flow. In sub-glacial tunnels, where melt water flows towards the ice-sheet margin, erosion of loose sediments and bedrock can be significant.

The topographic relief in Fennoscandia is generally not dramatic outside the Scandinavian mountains /e.g. Lidmar-Bergström and Näslund 2005/. The resistance to denudation of the Precambrian rocks that dominate in Fennoscandia is rather uniform, as compared with, for example, the variation between the Caledonian bedrock types in the Scandinavian mountains. Although the relief locally may be steep at many places, the relatively homogenous denudation resistance has contributed to the moderate to low relief of the Precambrian rock basement. The relative relief is exceptionally low (less than some tenths of m) along significant portions of the eastern Baltic coastline of southern and south-central Sweden due to the presence of the sub-Cambrian peneplain. This low relief favours low subaerial erosion rates, for example, the most important subaerial erosion process, fluvial erosion, increases with steeper topographical gradients.

4.6.4 Model studies/experimental studies

Some examples from Sweden of calculated denudation rates over long time periods can be found. Many of them use remnants of the *sub-Cambrian peneplain* as a reference surface. The sub-Cambrian peneplain is a denudation surface formed in crystalline rock with a typical relief of less than 20 m /Rudberg 1954, Lidmar-Bergström 1995/. It is interpreted to have been formed down to sea-level prior to the Cambrian. In eastern Småland and southern Östergötland, the maximum denudation of the tectonically uplifted sub-Cambrian peneplain is approximately 100 m. Weathering and stripping would have required a period of between 2 and 50 Ma to accomplish this denudation /Lidmar-Bergström et al. 1997/, once overlying sedimentary cover rocks had been removed. On the Swedish west coast, a so-called *Sub-Cretaceous etch surface* has been incised into the sub-Cambrian peneplain by weathering. In places, it has resulted in maximum bedrock lowering of 135 m. The time required for this amount of denudation was suggested to be between 3 and 68 Ma /Lidmar-Bergström et al. 1997/, with the denudation occurring during the Jurassic-Early Cretaceous. Finally, saprolite thicknesses of 50 m in Skåne were interpreted to have been produced over a time interval of 1–25 Ma /Lidmar-Bergström et al. 1997/.

Given the specific tectonic and climatic evolution, including phases of denudation, sedimentation, and stripping of saprolites, the above examples clearly show that the evolution of the sub-Cambrian peneplain in southern Sweden into incised younger types of landscape has been a very slow process, and that the total amount of material removed from the crystalline bedrock has not been large considering the very long time periods involved. The total maximum denudation of bedrock in areas of Precambrian basement in southern Sweden during the last 540 Ma is in the order of a few hundred metres. A significant part of this denudation took place during Mesozoic tropical conditions favourable for deep weathering.

During temperate conditions in Sweden, weathering only occurs where the bedrock is exposed. /Swantesson 1992/ has estimated the postglacial weathering of bare bedrock surfaces in southern Sweden during the Holocene to be less than 0.02 m. Weathering rates in tropical climates range between 2 and 48 m Ma^{-1} /Thomas 1994/. Although these weathering rates reported by /Thomas 1994/ have a large span, due to differences in temperature and humidity conditions, it can be seen that weathering is a slow process even under the most favourable tropical climatic conditions. Weathering of fresh bedrock under temperate climate conditions is a considerably slower process.

From studies of large scale bedrock morphology, /Lidmar-Bergström 1996/ estimated the total amount of glacial erosion during the Late Cenozoic glacial cycles on the pre-Cambrian basement rocks to be in the order of a few tens of metres, although with great variations. An estimate of the average amount of glacial erosion of the bedrock during the Quaternary period has also been provided by /Påsse 2004/. The study is based on the assumption that clastic sediments formed by the Scandinavian ice sheet remain within the glaciated area or at its periphery. If this is true, the volume of the sediments defines the average weathering and erosion depth of bedrock within the area. The average sediment depth in the area has been estimated to be 16 m, which corresponds to 12 m depth of fresh bedrock. Assuming that part of the sediments consist of glacially redistributed Tertiary regolith, the average glacial erosion of bedrock during a glacial cycle has been estimated to be about 1 metre.

Studies of glacial geomorphology can provide information on past glacial erosion. However, it is often difficult to date the geological information and thus to relate deposition or erosion events to a particular glacial phase. Model reconstructions of past glaciations can improve these interpretations and also aid in quantifying possible erosion depths in different areas. For example, /Näslund et al. 2003/ used an ice-sheet model reconstruction of the Weichselian glaciation to interpret geological information. In areas with relatively good geological datings, modelled ice flow directions are in good agreement with interpretations of field data, showing that such model results can aid in placing field data into a timeframe and chronostratigraphic context. A concept used in that study is *basal sliding distance*, which is defined as the time-integrated accumulated length of ice that has passed over the landscape by basal sliding. This entity can be used to estimate the spatial distribution of glacial erosion over the landscape. Calculations of basal sliding distances at the two candidate sites can be used together with local glacial geomorphology to investigate whether the amount of glacial erosion differs significantly from the averages estimated by /Påsse 2004/.

Given the expected climate-related conditions during the assessment period, with periods of temperate conditions, permafrost and glaciations, the physiographic conditions in Sweden and the characteristics of the bedrock in the Baltic Shield, it is highly unlikely that the suggested sites would experience denudation rates of more than a few metres in the coming 1 Ma.

4.6.5 Time perspective

Weathering, erosion and sedimentation are always active processes at the Earth's surface. In Sweden, the maximum total denudation can be expected to be limited in lowland areas of low relative relief, in the order of 1–10 m Ma^{-1} on average, but the rate of weathering and erosion can vary in time and space.

4.6.6 Natural analogues/observations in nature

As mentioned above, the current landforms in Fennoscandia are a result of the interaction between tectonic processes, weathering, erosion and sedimentation and consequently the traces of these processes can be observed and interpreted everywhere in nature. In Fennoscandia, large-scale bedrock landforms outside the mountain range, such as denudation surfaces and landscapes of weathering and stripping of saprolites, are common, and reflect the varying phases of weathering, erosion, and sedimentation that have occurred in association with tectonic events and climate change /e.g. Lidmar-Bergström 1996, Lidmar-Bergström and Näslund 2002/.

During the late Cenozoic glacial cycles, ice sheets have repeatedly covered parts or the whole of Fennoscandia, producing glacial erosional landforms in bedrock e.g. /Rudberg 1954/ and in surficial deposits e.g. /Kleman et al. 1997/. Traditionally, it has been thought that a considerable part of the bedrock relief is the result of glacial erosion. However, as mentioned above, it has been shown that the amount of glacial erosion of the Precambrian basement in general is in the order of a few tens of metres /Lidmar-Bergström 1996/. Valleys are more eroded than the surrounding terrain. Within the Scandinavian mountain range, valleys may have experienced several hundred metres of glacial erosion /Kleman and Stroeven 1997/. /Lidmar-Bergström, 1996/ further estimated that denudation occurring during the Proterozoic (600–2,500 million years ago) was in the order of tens of kilometres, and during the Mesozoic (65–245 million years ago) and Tertiary (2.5–65 million years ago) up to 600 m at the most. Furthermore, during the last decades our understanding of ice-sheet thermodynamics has showed that large portions of ice sheets may be cold-based and thus have a negligible erosive effect. Over the same period, numerous glacial geological studies have shown that the occurrence of preglacial saprolite remnants is solid evidence that ice sheets under certain circumstances cause very restricted glacial erosion, or even have a preserving effect of pre-glacial landforms /Lagerbäck 1988ab/ and /Kleman 1994/.

4.6.7 Handling in the safety assessment SR-Can

Present day knowledge on denudation processes suggests that denudation generally will be limited in lowland parts of Fennoscandia during the assessment period. Areas where the bedrock is highly fractured and weathering and erosion can be expected to be significantly more rapid than the estimated averages do not apply at the sites of interest. The impact of weathering and erosion on groundwater flow and rock stresses is considered to be insignificant over the time period of relevance in assessments. However, both processes will affect the evolution of the biosphere /SKB 2006h/ and the estimated doses to man. In a very long time perspective, several million years, weathering and erosion may somewhat alter topography and rock stresses by redistribution of sediments and rock mass. In an even longer time perspective, 100 million years or longer, the repository may be brought to the surface due to tectonic uplift in conjunction with a combination of denudation processes.

Current knowledge, for instance the work by /Swantesson 1992/, /Thomas 1994/, /Lidmar-Bergström 1996/, /Kleman 1994/ and /Påsse 2004/, supports the assumption that weathering and erosion are insignificant for repository safety in the time perspective of one million years. For the assumed temperate to glacial climate conditions, the degree of erosion is estimated to be in the order of metres during the next million years.

4.6.8 Uncertainties

Rates of weathering and erosion vary as environmental conditions change. The rate of weathering and erosion also depends on rock and sediment characteristics and topography. In spite of the uncertainties in future environmental conditions, there is no reason to believe that the weathering and erosion at the investigated sites should diverge significantly from the estimated averages. Both areas have a low relief with low topographical gradients, in turn producing limited fluvial erosion. Given the soil material and climatic conditions, wind erosion is likely to be insignificant.

Uncertainties in mechanistic understanding

There are uncertainties in the understanding of the detailed mechanisms of weathering and erosion. However, for the safety assessment, it is sufficient to estimate the amount of weathering and erosion of fresh bedrock during the assessment period.

Model simplification uncertainties in SR-Can

Not relevant for this process.

Input data and data uncertainties in SR-Can

Not relevant for this process.

4.7 Erosion/sedimentation in fractures

4.7.1 Overview/general description

During the construction, operation and early saturation phase of the repository, the rate of inflow of water from fracture zones towards the tunnels (and potentially to the backfill and to the bentonite buffer material surrounding the canisters) will increase. This increase might be large enough to: a) initiate erosion of fault gouge material, which accumulates by sedimentation further down-flow thereby changing the hydraulic conductivity of the zones, and b) may result in the erosion and removal of bentonite along the groundwater flow direction away from the deposition holes (i.e. a ‘flow-out’), resulting in a lowering of the bentonite density by dilution and a decrease of fracture conductivity where bentonite colloids sediment.

In terms of gouge material, its general friability will facilitate removal and transport, and there exists substantial quantities of gouge in some of the major, most transmissive fractures at the sites being investigated by SKB.

As to bentonite, following closure of the repository, it will gradually become saturated and undergo swelling and any remaining openings will be sealed. This will also include the plugging (by a clay gel material) of open (and sometimes hydraulically active) fractures that have been transected by the deposition hole /Pusch 1983/. Although the deposition holes will be positioned to avoid, as far as possible, any significant water-conducting fracture systems, it will be inevitable that some will be present. Furthermore, any tectonic activity that might occur during the lifespan of the repository may widen existing fracture zones, rendering them more hydraulically active, or even induce new ones. Piping/erosion and chemical erosion of bentonite is further described in the Buffer/backfill process report /SKB 2006g/.

In general, the rate of inflow of water towards the tunnels during excavation, operation and post-closure saturation will not be high enough to cause significant erosion/sedimentation. Very conductive fractures, where erosion/sedimentation could be induced by the excavation, will be grouted, since depression of the water table most probably will be regulated by construction licenses, and to avoid upconing of saline waters as this is not desirable for the performance of the backfill.

4.7.2 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-Can is also indicated in the table and further described in Section 4.7.7.

4.7.3 Boundary conditions

The conditions at the geosphere boundaries that influence erosion/sedimentation processes in fractures are groundwater pressures; they will cause the required flow of groundwater for erosion to take place.

4.7.4 Model studies/experimental studies

Various clay forms have been laboratory tested for their erosion properties using the 'pinhole test' /Pusch 1983/ see also the Buffer/backfill process report /SKB 2006g/. The erosion of the clay gel in the fracture zone depends on the shear strength of the clay as well as on the flow rate of water in the fractures, this rate being determined by their apertures and by the local hydraulic gradient. Experience from the Stripa Buffer Mass Test /Pusch et al. 1982/ indicates that, under normal circumstances, erosion and removal of bentonite clay is not expected to be an important process during the repository lifespan.

If, long time after resaturation, large-scale shearing resulted from tectonic activity, then the softer clay gel at the fracture opening would be removed but the main stiffer bulk of the bentonite seal is expected to remain intact /Pusch 1983/ see also the Buffer/backfill process report /SKB 2006g/.

4.7.5 Time perspective

Erosion/sedimentation in fractures is only of potential significance while relatively large groundwater flows occur during the initial stages of the repository life (excavation, operation and re-saturation periods).

4.7.6 Natural analogues/observations in nature

No analogue studies have been specifically focussed on these erosion/sedimentation phenomena.

Table 4-6. Direct dependencies between the process "Erosion/sedimentation in fractures" and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	No.	–	–	No.	–.	–
Groundwater flow	Yes.	All.	Process neglected; site observations indicating limited significance at repository depth.	No. But, indirectly by changing the fracture geometry.	–	–
Groundwater pressure	Yes.	All.	Process neglected; see row Groundwater flow above.	No. But, indirectly by changing the fracture geometry.	–	–
Gas flow	Yes. But expected gas flow is too low to accomplish erosion.	All.	Process neglected; see row Groundwater flow above.	No. But, indirectly by changing the fracture geometry.	–	–
Repository geometry	No. But indirectly through changes in the ground-water flow induced by the repository geometry.	–	–	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	No.	–	–	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.	–	–
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.	Process neglected	No.	–	–

4.7.7 Handling in the safety assessment SR-Can

Changes of conductivity in fractures over time are not addressed in SR-Can. In particular, erosion and sedimentation in fractures due to natural processes during a glacial cycle are not considered in SR-Can. The amounts of fracture-filling minerals and gouge material found nowadays in the most transmissive fractures at the investigated sites indicate that these processes are of limited significance at repository depth. It is further expected that grouting, which is needed to avoid pronounced depression of the water table at the repository site during the operation/excavation phase, will also ensure that erosion and sedimentation does not occur in the fractures influenced by the repository.

4.7.8 Uncertainties

Uncertainties in mechanistic understanding

The erosion/sedimentation process is well understood.

Model simplification uncertainties in SR-Can

Not relevant. Modelling of this process is not thought to be necessary. Furthermore, no models have been identified to estimate the effects of erosion/sedimentation in fractures.

Input data and data uncertainties in SR-Can

Not relevant.

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 chemical, whereas other processes are in 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". In the strict sense, mixing is not a process. 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 counterparts Fe^{3+} and U^{4+}. 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 from/to the biosphere, and by exchange with very deep-lying groundwater. 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 long-term climate change, which leads to altered precipitation 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 historical evolution, i.e. the conditions that have given rise to today's situation. The site descriptive models of the Forsmark area and the Simpevarp/Laxemar subareas /SKB 2005ab, 2006a/ 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 isolated. Even in a situation where the isolation 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 /SKB 1995/.

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 causes pitting, whereas sulphide corrosion is distributed evenly over the whole surface. Absence of oxygen 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 undermine 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 process report /SKB 2006g/). 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 process report /SKB 2006g/). 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 Advection/mixing

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 the groundwater. The process 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.

Section 3.1 describes the processes that control the groundwater flow through the fractured rock in the geosphere.

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 velocity. The mean transport velocity of the water particles, or any inert particle transported by the flowing water, is obtained as the Darcy velocity divided by the flow porosity. This resultant transport process describes the bulk movement of the groundwater and is called advection.

The Darcy velocity 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, seasonal variations (rainfall, ground freezing and snowpack development). 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.

It may 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 in the strict sense not a process but an aggregate result of spatially variable advection and diffusion. Groundwater moves by advection in connected flow paths of the rock's fracture system. These meet, to a greater or lesser extent, so that 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 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 large proportions of water originating from colder climatic conditions are generally found down to a level of 100–300 m. 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. However, it is assumed that the last glaciation had the largest impact on the present groundwater composition. Most of the groundwater from the previous deglaciations should have been flushed away in the case that 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. 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 the 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.

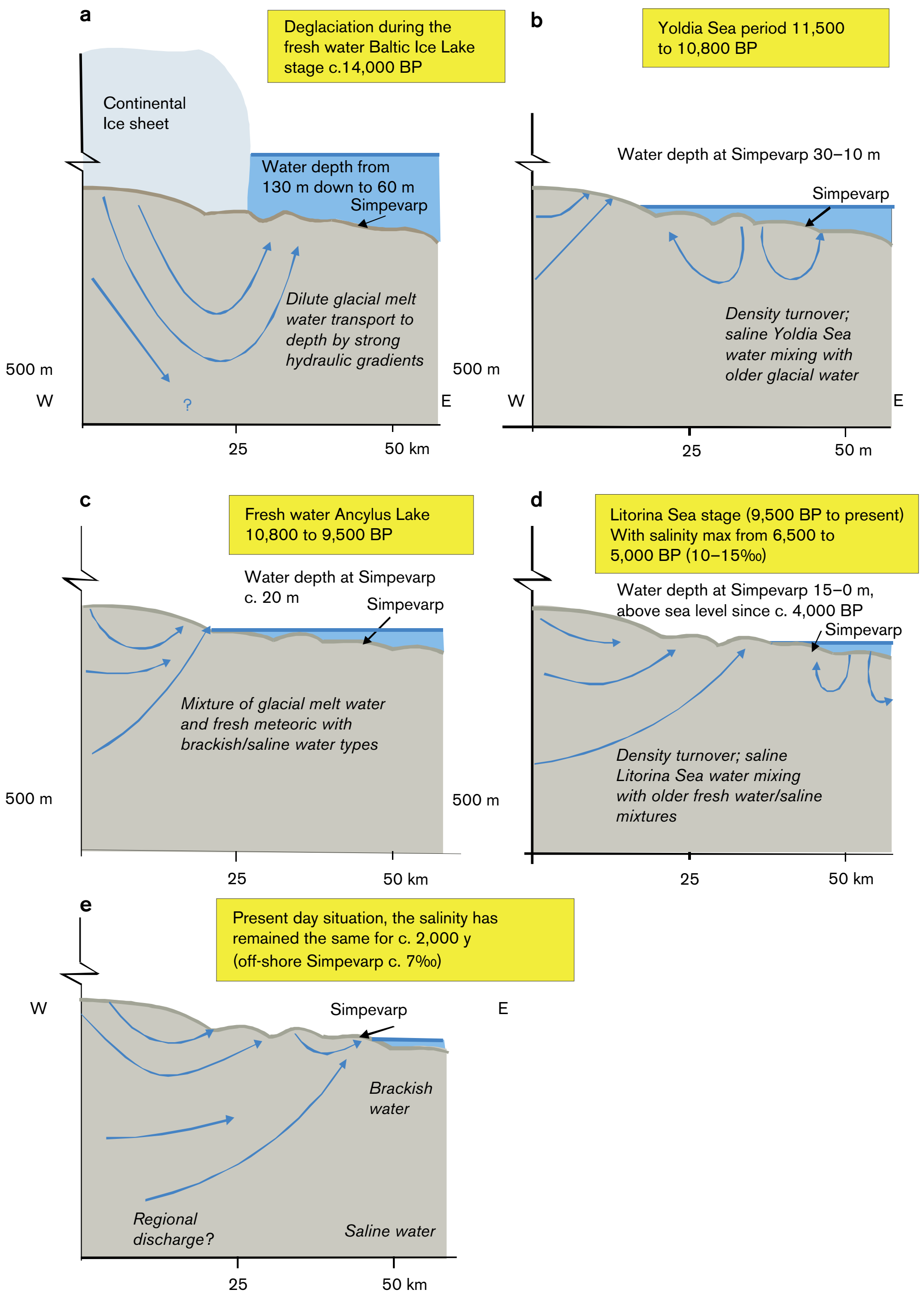

***Figure 5-1.** Conceptual model of the evolution of the Simpevarp subarea from the retreat of the ice after the most recent ice age until today. The different stages of the Baltic Sea are of great importance for the large-scale groundwater flux at the three sites. The difference between the sites is greatest during the period from the Littorina stage up to present-day situation /SKB 2004d/.*

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 brine, i.e. either a very saline water where the salt has been leached out of the rock over millions of years or a saline water originating in seawater freezing, and there may even be an external component of some ancient residual basinal brine.

Mixing is thus a process which is essentially controlled by external climate 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 from precipitation (meteoric water), saline water under permafrost, glacial meltwater and, in areas below the highest shore-level, 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.

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-Can is also indicated in the table and further described in Section 5.2.7.

Table 5-1. Direct dependencies between the process "Advection/mixing" and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	No. But indirectly through groundwater flow.	–	See Section 3.1.	No. But indirectly minor influence through groundwater flow.	–	–
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).	–	See Section 3.1.
		Temperate	Transport of salinity included in groundwater flow modeling (Section 3.1). Flow field from hydrogeological modelling used in calculations of advective transport of radionuclides, see Section 6.1.			
		Permafrost	Transport of salinity from beneath a permafrost layer to repository depth included in groundwater flow modelling, see Section 3.1.			
		Glaciation	Upconing of saline water and transport of glacial meltwater included in groundwater flow modelling, see Section 3.1.			
Groundwater pressure	No. But indirectly through groundwater flow.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Gas 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.	–	–
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	Transport of salinity included in groundwater flow modelling, see Section 3.1.
					Temperate	Distribution of salinity from hydrogeology modelling. Assessment of water composition based on output from hydrogeology modelling. See Section 3.1.
					Permafrost	Transport of salt from beneath a permafrost layer to repository depth included in groundwater flow modelling, see Section 3.1.
					Glacial	Upconing of saline water and transport of glacial meltwater included in groundwater flow modelling, see Section 3.1.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Gas composition	No.	–	–	No. But indirectly through ground-water 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 change 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 velocity 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 *á priori* for the advective and dispersive transport based solely on hydraulic data such as flow rates and pressures. Specifically, for estimating the time scale 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, a scale dependence has been observed for the 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. 2002, Poteri et al. 2002/.

The Simpevarp, Forsmark and Laxemar sites are being 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. 2005ab, SKB 2005ab/. Groundwater chemical data are analysed using, among others, mixing models /SKB 2004d/.

The importance of mixing for 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 /Parkhurts 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 on Äspö 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/. The results indicate that mixing has occurred in several phases as a result of varying flow conditions. Since the most recent ice age the following mixing processes have been identified and quantified (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 (7,000 years ago) 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 Äspö rose above sea level about 3,000 years ago.

This sequence of events probably occurred many times during past glaciation cycles. Most of the glacial meltwaters 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, e.g. glacial meltwaters, probably originate from the most recent event, i.e. the last ice age.

A hydrodynamic simulation of these conditions for the Äspö site has been carried out by /Svensson 1999/. Similar modelling is performed for the sites being investigated by SKB /Hartley et al. 2005ab, Follin et al. 2005ab/. 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 Äspö site, the sequence of dominant waters at 450 m depth is: glacial meltwater (at the start of the numerical simulation), Yoldia Sea water, Ancylus Lake water, Littorina Sea water and, finally, today's meteoric water. 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 suggests 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 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, permafrost 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.

As regards modelling of the radionuclide transport, advective travel times from repository sites up to the biosphere of the order of tens to hundreds of years have typically been obtained /Walker and Gylling 1998, 1999, Gylling et al. 1999/. Dispersion does not significantly influence these time spans. It is important to note that these advective travel times are pure model results without any counterpart in the actual systems; an actual "water particle" is subjected to both diffusion and matrix diffusion (see below) and thereby has a longer travel time. Furthermore, the travel times cited above are proportional to the assumed porosity, which is not well known in fractured rock (see "Summary of uncertainties" below).

5.2.6 Natural analogues/observations in nature

Several tools, such as the M3 computer model /Laaksoharju et al. 1999b/, 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 et al. 2001b, Pitkänen et al. 1998, 1999, 2004/, it has been possible to distinguish the effects of mixing from the effects of chemical reactions. In the model study for Oklo, the described flow conditions could subsequently be verified by hydrogeological models.

As mentioned above, data from the site investigations at Simpevarp, Forsmark and Laxemar are being modelled for advection-dispersion, matrix diffusion and density driven flow, see e.g. /Hartley et al. 2005ab/, and groundwater chemical data are analysed using, among others, mixing models /SKB 2004d/.

5.2.7 Handling in the safety assessment SR-Can

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 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 previous chemical and hydrological conditions. The descriptions can be divided into the period when the disturbance of the repository influences advection and mixing and the following initial and future periods of temperate, permafrost and glacial domains when shore-line displacement, development of permafrost and advance and retreat of ice sheets control advection and mixing.

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. These calculations are based on the principles of reference waters and their transport as described above.

Temperate period

In Section 3.1, the groundwater flow modelling for the temperate period 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.

Permafrost and glaciation periods

During the next 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 will be made based on the climate domains (see SR-Can Climate report, Section 1.4 /SKB 2006e/).

In Section 3.1, the groundwater flow modelling for the permafrost period is described. The main issue related to advection and mixing that is considered is the transport of highly saline water from beneath the permafrost layer to repository depth.

During periods of the glacial domain, water with low ionic content may be brought down and cause the bentonite to form colloids. The opposite extreme is that very saline water is brought up to repository level and reduces the buffer's swelling capacity. In Section 3.1, modelling of groundwater flow during the glacial domain is described. Specifically, upconing of saline water and transport of glacial meltwater to repository depths are addressed in the modelling.

Of special importance during the glacial domain is the possible transport of oxygenated water down to repository level. The conditions then differ from today's in that there may not be any 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-Can using advective travel times from the glacial modelling. Calculations carried out /Guimera et al. 2006, Sidborn and Neretnieks 2006/ show that the quantity of oxygen that can be transported in this way is limited and that the rock has the capacity to consume this oxygen. Microbial processes are expected to influence the rate of oxygen consumption, see Section 5.6.4.

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-Can

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 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 capacity 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 ten to a hundred years in the uppermost 100 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. /SKB 2004d/. At greater depths, more than 1,000 m, the residence times are much longer, see e.g. /Louvat et al. 1999/.

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 on Äspö since the island rose above the surface of the sea approximately 3,000 years ago. 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 isostatic uplift.

Input data and data uncertainties in SR-Can

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-Can are discussed at length in the underlying site-descriptive modelling reports /SKB 2005ab, 2006a/.

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 and Skårman 1995, Laaksoharju et al. 1995b, Laaksoharju et al. 2004ab, SKB 2004d/.

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.

5.3 Diffusion and matrix diffusion

5.3.1 Overview/general description

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 in the rock may enter these pores through diffusion, a phenomenon known as matrix diffusion.

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/. Most of the text below is taken directly from /RETROCK 2005/ and from 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, especially for sorbing radionuclides that, through matrix diffusion, have access to the very large inner surfaces of the rock matrix. These surfaces can typically be 3 to 6 orders of magnitude larger in area than the surfaces of the fractures where the water flows.

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. For non-charged species, 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_f (–). 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. The storage capacity of the rock matrix ($\alpha = \varepsilon + K_d\rho$) is the combined storage capacity due to dissolved species in the pore water and interaction of species with mineral surfaces by sorption. The key entity for storage of non-sorbing solutes in the pore water is the porosity ε (–).

Mineral surfaces are most often negatively charged under natural groundwater conditions; thus there is a repulsion of negatively charged ions close to the surfaces. For very small pores, this means that anions are excluded from an important fraction of the pore space resulting in a smaller effective 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. Anion exclusion is believed to be of less importance in crystalline rock compared with other geological host media. The effect is more pronounced in groundwater at low ionic strengths than in highly saline waters.

Surface diffusion has been proposed as a process explaining observations of increased diffusion rates for some cations. This means that sorbed radionuclides may be affected by concentration gradients and thus become 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 assessment, which is regarded as a conservative approach, since an increased diffusivity in the rock matrix would increase the retention in the geosphere.

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 occur. 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).

The stability of the matrix pore system over longer time periods is a crucial and difficult question. Alterations in the flow field due to geological and climatic alterations may change the fractures or parts of a fracture surface where matrix diffusion is possible. Precipitation and dissolution of mineral phases may be caused by changes in water composition from natural causes or by materials introduced in the repository. Changes in mineral phases may affect the available transport porosity both in the fractures and in the rock matrix.

Domains of a fracture plane can contain more or less stagnant water. Diffusion into stagnant zones has been used to explain pronounced tailing in the breakthrough of short-term experiments that could not be explained by diffusion into the rock matrix. Diffusion into stagnant zones is generally treated as a short-term process with limited capacity. At longer time scales, diffusion from stagnant zones into the matrix of the adjoining rock can provide further retention.

In addition to being of importance for radionuclide retention, matrix diffusion plays a role in the long-term evolution of hydrogeological conditions at a potential repository site. In saline groundwaters, diffusion of salt between the flowing groundwater and the immobile groundwater in the rock matrix may affect groundwater flow through changes in water density (see Section 3.1). However, there is yet no clear experimental evidence that diffusion has been, or will be, significant for groundwater composition at repository depth.

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-Can is also indicated in the table and further described in Section 5.3.7.

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 the report by /Liu et al. 2006/ as support to the recommendation of diffusion data for SR-Can. Some examples from the report by /Liu et al. 2006/ 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 and Switzerland, mostly in the 1980's. In addition to providing diffusivities and formation factors of the rock matrix, the results of these studies indicate that fracture-filling minerals have higher diffusivity than the host rock and that the diffusivity or formation factor is lower in samples under stressed conditions /Bradbury and Green 1986, Skagius 1986/.

Field-scale tracer diffusion experiments at 360 m depth in the Stripa mine in Sweden have shown that micropore connectivity extends to at least 40 cm /Birgersson and Neretnieks 1988, 1990/. The results also indicated large variability in the diffusivities evaluated from the experiments, despite a relatively homogeneous rock matrix.

Table 5-2. Direct dependencies between the process “Diffusion and matrix diffusion” and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	**Time period**	**Handling of influence**	**Influence present?**	**Time period**	**Handling of influence**
Temperature in bedrock	Yes. But the variation is small in the expected temperature range.	All.	Diffusion coefficients at constant T.	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 P.	No.	–	–
Gas flow	No.	–	–	No. But indirectly through water composition (dis-solved gases which may subsequently come out of solution.	–	–
Repository geometry	No.	–	–	No.	–	–
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. The 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 in groundwater flow modelling. Geometry of flow paths and matrix porosity, see Section 6.1.			
		Permafrost	Generic calculations of salt advection and matrix diffusion performed on a description of fracture and fracture zone geometry for Laxemar see Section 3.1. Transport of radionuclides, discussed in Section 6.1.			
		Glaciation	See Permafrost above.			
Rock stresses	No. But indirectly through changes in fracture/pore geometry.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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.	–	See Section 5.6.
Groundwater composition	Yes. Concentration gradients are the driving force for diffusion.	Excavation/ operation	Modelling of salinity driven flow and matrix diffusion included in hydrogeological modelling, see Section 3.1.	Yes.	Excavation/ operation/ resaturation	Results from hydrogeological modelling on salinity in fractures and rock matrix, see Section 3.1.
		Temperate	Exchange of salt between mobile and immobile water included in groundwater flow modelling, see Section 3.1. Transport of radionuclides, see Section 6.1.		Temperate	Effects on salinity of exchange of salt between mobile and immobile water included in the groundwater flow modelling, see Section 3.1. Transport of radio-nuclides, see Section 6.1.
		Permafrost	Exchange of salt between mobile and immobile water included in the generic modelling of groundwater flow see Section 3.1. Transport of radionuclides, see Section 6.1.		Permafrost	Effects on salinity of exchange of salt between mobile and immobile water included in the groundwater flow modelling, see Section 3.1. Transport of radio-nuclides, see Section 6.1.
		Glaciation	See Permafrost above.		Glaciation	Same as for Permafrost 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.	–	–
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.	–	–

Based on the analogy between the diffusion process and the electrical conductivity process in pore water, in situ electrical conductivity borehole logging has been conducted in granitic rocks to determine diffusion properties /Löfgren et al. 2001, Löfgren and Neretnieks 2002, 2003, Löfgren 2004/. These results indicate that the unaltered rocks have micropore connectivity up to metres. In addition, open fractures with stagnant water and alteration zones around fractures are found to have increased electrical conductivity in the down-hole measurements.

Both laboratory experiments and in situ electrical conductivity loggings in boreholes are conducted as part of the site investigation programme at Forsmark and Simpevarp/Laxemar. The results for Forsmark, where the rock stresses are high, show a clear discrepancy between field and laboratory tests. This indicates that the stress-released samples might not be representative for in situ conditions.

5.3.5 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.

5.3.6 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 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/. The measured concentration profiles 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/.

5.3.7 Handling in the safety assessment SR-Can

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 period

The hydrogeological modelling undertaken for the temperate period represents variable-density flow due to variations in salinity. In this modelling, diffusion of several groundwater constituents, e.g. chloride, between flowing groundwater and immobile groundwater is included, see Section 3.1.7. Thus, in addition to providing the groundwater flow conditions, the results can be used to explain 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 fracture is handled via the transport resistance. Matrix diffusion is coupled to sorption via the concentration of the solute in the porewater and this coupling is handled by the K_d approach (see Section 5.4.7). The integrated modelling approach is further described in Section 6.1.7.

Permafrost

The possible movement of saline waters arising from salt exclusion during freezing beneath the permafrost layer to greater depths due to density effects will be studied. Both the depth of the salt front and corresponding transport times are of interest. These issues are addressed by hydrogeological simulations (DarcyTools code) where exchange of salt between mobile and immobile groundwater is considered, see also Section 3.1.7.

Since the upper part of the geosphere may be frozen and place considerable restrictions on flow, no detailed radionuclide transport calculations are carried out for permafrost conditions. However, bounding calculations are undertaken in order to estimate radionuclide dose levels, see further Section 6.1.7.

Glaciation

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) after a glaciation and reactions between oxygen and rock minerals will be 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.

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 pore water can be assumed.

Model simplification uncertainties in SR-Can

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 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-Can will be as given above, i.e. to consider matrix diffusion for the host rock only.

The main uncertainty related to matrix diffusion in the hydrogeological modelling is the same as in the radionuclide 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-Can

Input data and associated uncertainties for quantifying matrix diffusion in the integrated radionuclide transport modelling are compiled in the SR-Can data report /SKB 2006d/. In addition to matrix diffusivity, 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 in the supporting report by /Liu et al. 2006/ as well as on the site-descriptive models for the Forsmark area and the Simpevarp/Laxemar subareas /SKB, 2005ab, 2006a/.

5.4 Speciation and sorption

5.4.1 Overview/general description

Two recent compilations of information on sorption phenomena and their representation in performance assessment applications have been produced in connection with SKB's programme. First, in the EU concerted action project RETROCK, a status report on sorption modelling has been presented /RETROCK 2004, 2005/. Second, as part of the production of the SR-Can Data report /SKB 2006d/, the scientific basis for sorption and modelling of sorption has been evaluated /Crawford et al. 2006/. Much of the information below is based on these two compilations.

The term "sorption" includes a number of different retention processes/mechanisms for interaction between substances (e.g. radionuclides) that are transported dissolved in groundwater and the solid surfaces of the rock. In the following, the focus is on sorption of radionuclides, and hence the term radionuclide is used rather than the general term solute. However, the sorption processes discussed apply to solutes in general. Sorption as a term describes the process of attachment of dissolved species to mineral surfaces. Although Van der Waals interactions are also possible, sorption is mainly considered as attachment by stronger electrostatic and chemical bonding. The most important mechanisms are ion exchange and surface complexation /Carbol and Engkvist 1995/.

Sorption can take place directly on the surfaces of the water-bearing fractures or on the surfaces of the microfractures inside the rock matrix, where the water is more or less stagnant. Furthermore, sorption can take place on other materials, such as clay minerals, which may be present on the surfaces of the water-bearing fractures.

Depending on the process in question, the strength of the sorption is highly dependent on the chemical properties of the ions and the presence of possible complexing agents. Therefore, it is essential to know the redox conditions, and the groundwater's pH and content of complexing agents such as humic and fulvic acids. The chemical form of the radionuclide (speciation) is controlled by the prevailing redox conditions. Complexation in the aqueous phase can reduce the sorption for some radionuclides. The amount of the reduction depends upon the chemical properties of the radionuclide concerned and the types of complexing agents present and their properties. The chemistry of simple complexing agents such as dissolved carbonate is well described theoretically and can be accounted for with relative ease. More complex ligands such as humic and fulvic substances can also be accounted for although 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 likely to be of only limited importance. In connection with ion exchange, the salinity of the water is also of great importance. High salinity reduces the sorption of e.g. Cs^+ and Sr^{2+} /Carbol and Engkvist 1997/.

The minerals that serve as the substrate for sorption have different capacities for taking up radionuclides. Some minerals are, for example, strong ion exchangers, whereas others are not. Clay minerals and iron oxyhydroxides have a large capacity to bind radionuclides. Also, competition for sorption sites between radionuclides and major groundwater constituents may reduce the radionuclide retention. Moreover, isotopic dilution may reduce the sorption of radionuclides, but is generally not considered to be an issue of concern due to the low concentrations of radionuclides in the geosphere far-field. An exception may be e.g. Cs^+ where the natural concentrations of stable Cs^+ may imply reduced sorption of the radioactive Cs^+ due to non-linearities in the sorption isotherm.

A number of other processes besides ion exchange and surface complexation also influence the distribution of radionuclides between the aqueous phase and solid phase. Precipitation reactions and co-precipitation (mineralisation) have been proposed as processes that can contribute to the retention of radionuclides /Bruno 1997/. These processes, which are highly dependent on the speciation of the radionuclides and the saturation of the water with respect to the minerals in question, are, however, not usually regarded as sorption reactions. Sorption as a first step in forming solid solutions is treated as precipitation and coprecipitation /RETROCK 2004/.

Sorption of some radionuclides can be irreversible in practice and then results in permanent immobilisation of the radionuclide. In these cases, the radionuclide is incorporated in the mineral lattice. For radionuclides that have the potential to be immobilised, the sorption capacity of the geosphere can be considered unlimited given the amount of these radionuclides, i.e. the sorption will not be weakened as the amount of sorbed material increases.

Not only the chemical conditions in the water (notably pH, redox and salinity) but also temperature and pressure determine what speciation (chemical form) the radionuclides will have. The importance of chemical speciation lies in its control of the geochemical reactions likely to occur and the 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-Can is also indicated in the table and further described in Section 5.4.7.

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 has been described according to several models. A first group of models are empirical: they only describe by means of coefficients the experimental partition between the solute in solution and the solute adsorbed (the K_d approach). Another group of models aims to represent the mechanism of the sorption reactions with a thermochemical formulation (thermodynamic sorption models, or TSM). These are the surface complexation and the ion exchange models.

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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes. A temperature dependence exists (2nd and 3rd laws of thermodynamics).	Excavation/ operation Temperate Permafrost Glaciation	Process neglected for radionuclides. Use of Kd approach; data at constant temperature.	No.	–	–
Groundwater flow	No. But indirectly by affecting water composition. Also, If sorption is kinetic, groundwater flow (water velocity) controls sorption.	–	–	No.	–	–
Groundwater pressure	Yes. Affects chemical speciation.	All	Influence neglected; little significance compared with other influences.	No.	–	–
Gas 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 Temperate Permafrost Glaciation	Process neglected for radionuclides. Geometry of flow paths, see Process 6.1. Site-specific porosities, BET surfaces and stress effects considered in the selection of Kd. Surface retardation neglected.	No. Only if precipitation is considered, aperture could be changed.	–	–
Rock stresses	No. But indirectly through changes in fracture/pore geometry.	–	–	No	–	–
Matrix minerals	Yes. Mineralogy important for sorption mechanisms.	Excavation/ operation Temperate Permafrost Glaciation	Process neglected for radionuclides. Site-specific minerals and BET surfaces considered in the selection of Kd values.	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.
Fracture minerals	Yes. Mineralogy important for sorption mechanisms.	Excavation/ operation Temperate Permafrost Glaciation	Process neglected for radionuclides. Site-specific minerals and BET surfaces considered in the selection of Kd values. However, surface retardation neglected.	Yes. Precipitation/co-precipitation may change fracture surface properties when trace elements are incorporated into mineral structure.	All	Effect neglected (precipitation effects not accounted for). Also, sorption on fracture surfaces not accounted for, see Section 5.4.7.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Groundwater composition	Yes. Speciation, pH effects, salinity effects etc.	Excavation/operation Temperate Permafrost Glaciation	Process neglected for radionuclides. Salinity, pH, redox, organic acids, microbes considered in the selection of Kd values.	Yes. Uptake of trace elements controls concentration in water phase.	Excavation/operation Temperate Permafrost Glaciation	Process neglected for radionuclides. Sorption of radionuclides and trace elements not accounted for when main elements determined. For radio-nuclides, see Section 6.1.
Gas composition	No. But indirectly through dissolution of gas changing water composition.	–	–	No. But indirectly since water phase concentration controls gas phase concentration.	–	–
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 Permafrost Glaciation	Process neglected for radionuclides. Sorption of radionuclides considered for saturated conditions only.	No.	–	–

A large number of experimental, radionuclide-specific studies of sorption have been carried out /Carbol and Engkvist 1995/. These are usually conducted as batch tests where a specimen containing the radionuclide in question in aqueous solution is allowed to come to equilibrium with the solid rock material. Minerals and water compositions are used to represent the typical spatial variability for the repository site and the important parameters – such as pH, ionic strength and concentrations of radionuclides – are then varied. The change in the aqueous concentration of the radionuclide provides a measure of the sorption. Column tests with flowing water can also be used to estimate the sorption. In the field, attempts have been made to estimate the sorption directly by determining the distribution of a tracer between fracture surfaces and equivalent groundwater in boreholes /Landström and Tullborg 1990/. Transport experiments with sorbing tracers in the field can also be used to estimate the strength of the sorption process /Frick et al. 1992, Winberg et al. 2000/. In addition, sorption properties can be evaluated from in-diffusion and through-diffusion experiments in intact rock pieces, e.g. /Byegård et al. 1998/.

If the sorption is linear, completely reversible and in equilibrium, a distribution coefficient, K_d, for the particular water chemistry in question can be estimated. The assumption of linearity is usually met at the low concentrations that are of interest, and the assumption of equilibrium is met if the sorption has a timescale that is much shorter than the timescale for transport by advection and dispersion. The use of K_d entails a simplification of the relatively complex sorption processes. Models that take into account non-linear sorption and/or non-equilibrium conditions exist, but are seldom used in safety assessments.

5.4.5 Time perspective

For most radionuclides, the sorption process, particularly ion exchange, is considered to be fast compared with the timescale for advective transport in fractured rock. This means that equilibrium between rock material and aqueous phase usually prevails under natural conditions.

Processes such as incorporation of radionuclides in the mineral lattice are much slower than ion exchange and cannot be considered to be in equilibrium with the rock. However, these processes are not utilised directly in the safety assessment (see below).

5.4.6 Natural analogues/observations in nature

Sorption as a reversible equilibrium process is hard to observe in nature. However, (more or less) irreversible sorption processes are easier to observe, and can be studied on rock fragments. Examples include Poços de Caldas, El Berrocal, Cigar Lake, Grimsel and Oklo /Miller et al. 2000/.

Sorption can in principle be studied in tracer experiments in which resin injection “freezes” the flow field such that radionuclides cannot move away from their sorption sites. Such experiments have been performed at the Grimsel test site /Möri et al. 2000/ and are also planned within the TRUE continuation programme.

Coprecipitation and surface precipitation can be studied in nature more easily. Coprecipitation has been extensively applied in analytical chemistry for the separation of trace elements, enrichment processes and mixed-oxide fuel production /Bruno and Sandino 1988, and references within/. There are also extensive data on the coprecipitation of radionuclides with calcite /Curti 1999/. A compilation of studies on natural analogues regarding the mechanisms controlling the aqueous concentrations and speciation of several elements are given in /Bruno et al. 2002/.

5.4.7 Handling in the safety assessment SR-Can

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 back-filled tunnels go from zero to full saturation.

No radionuclide transport is expected to occur during this phase.

Temperate period

The simulation of an approximately 10,000 year long period (initial temperate period) extending from after repository closure (or rather re-saturation) up till the initiation of the next permafrost-glaciation event is undertaken. However, the calculation of doses may extend up to a million years.

For sorption, it is assumed that a simplified linear equilibrium model (utilisation of K_d) is applicable for safety assessment. This approach implies that retention processes such as surface precipitation and co-precipitation are not considered in the safety assessment.

In order not to overestimate sorption in connection with changes in water chemistry, cautiously pessimistic distribution coefficients are assigned /Carbol and Engkvist 1995, 1997, Crawford et al. 2006/. In SR-Can, different values of K_d are used for non-saline and saline water, and in relevant cases for different redox forms. In principle, K_d can also be compensated for a decrease in sorption caused, for example, by humic and fulvic acids /Grenthe et al. 1992/, and by microbial effects, see Section 5.7. However, an uncertainty span for K_d is used in SR-Can that includes both experimental uncertainty and uncertainties regarding the natural chemical environment. For further discussion of parameters values in SR-Can, the reader is referred to the SR-Can Data report /SKB 2006d/ and /Crawford et al. 2006/.

Permafrost and glaciation

No detailed radionuclide transport calculations are carried out for permafrost and glacial conditions. However, bounding calculations are undertaken in order to estimate radionuclide dose levels, see further Section 6.1.7.

5.4.8 Uncertainties

Since sorption is a collective term for several processes, it can be claimed that our conceptual understanding varies. The use of the simplification with the distribution coefficient K_d is conceptually and practically attractive, but the validity of this approach can be questioned under certain specific conditions when the prerequisites of the concept (linearity, reversibility and equilibrium) are not fulfilled. However, 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 a non-linearity for some elements. Thus, the validity of the concept does not in itself entail an uncertainty factor, given the purpose of the safety assessment.

The greatest single uncertainty factor that affects the K_d value is the variability of the groundwater chemistry /Bruno and Duro 1997/. Given all uncertainties, the K_d values that are used in safety assessments (see below) are chosen so that the retention capacity in radionuclide transport is not overestimated, i.e. cautiously pessimistic values are used.

Sorption by means of surface complexation can theoretically also be described with surface complexation models. These models are general and well-founded, but require a large quantity of thermodynamic data for the sorbing substances. Furthermore, they require surface complexation constants, which are difficult to measure for all possible combinations of radionuclides and minerals. Therefore, the results of different experiments with surface complexation models have not been used to replace the distribution coefficients (the K_d values), but rather to further increase our understanding of the sorption mechanisms and determine what they are dependent on, i.e. how reliably estimated the sorption can be considered to be /Carbol and Engkvist 1995, Olin and Lehikoinen 1997/.

Uncertainties in mechanistic understanding

The recent literature review by /Crawford et al. 2006/ indicates that a great number of breakthroughs have been made in the last decade on almost every level concerning the state-of-the-art with regard to sorption modelling. Many of the modelling approaches that were proposed from the mid 1970's to the late 1980's suffered from a lack of experimental data and supporting evidence to allow for their use in practical applications. Since then, a large number of datasets have been generated for different pure mineral systems and occasionally for heterogeneous mixtures of minerals.

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 values are, indeed, cautious in a performance assessment framework. Additional work will need to be done to examine and reinterpret existing data to assess effects of e.g. enhanced sorption due to crushing, effects of contact time, and effects of water composition. Furthermore, there is some evidence in the existing data to suggest that K_d-values may be underestimated when neglecting diffusion effects. This, however, is not a big concern in performance assessment, as the data will be cautious with respect to what would be measured under true equilibrium conditions.

More worrying is that the use of crushed material in laboratory sorption experiments results in the creation of new surfaces for sorption (relative to intact rock) that cannot be quantified in a satisfactory and unambiguous manner. This raises the possibility that the K_d-values derived from laboratory experiments on crushed material may be overestimated and thus, not cautious in a performance assessment framework.

As a direct consequence of this, there is still a large amount of uncertainty concerning how best to extrapolate sorption properties derived from laboratory experiments conducted on crushed material to that of intact rock under in situ conditions. It is further noted that even measurements on whole rock pieces in the laboratory may be biased due to unloading effects.

Model simplification uncertainties in SR-Can

A representation of sorption with a K_d approach implies some uncertainties. First, the K_d values are in some respect chosen cautiously, thus not providing a true prediction of the transport. Also, the fact that immobilisation processes such as surface complexation and co-precipitation are not included implies that realism is lost. Moreover, subsequent dissolution of solid phases containing radionuclides, if chemical conditions change, is not described.

An attempted effort to address these shortcomings in SR-Can is done through process-based retention and transport modelling, where a more realistic description of retention phenomena is pursued. The process-based modelling mainly serves as a means to understand and quantify the uncertainties implied by the simplified K_d approach. An example of this type of modelling is surface complexation modelling trying to predict the outcome of the sorption measurements within the site investigation programme /Höglund et al. 2006/.

Input data and data uncertainties in SR-Can

The input data are discussed in detail in the SR-Can Data report /SKB 2006d/ and in the supporting report /Crawford et al. 2006/. The data compilation in /Crawford et al. 2006/ is based on the site-descriptive transport models and other pertinent data such as the SR 97 data collection /Carbol and Engkvist 1997/. However, the final uncertainty assessment and choice of parameter values for the calculations within SR-Can is made directly in the Data report /SKB 2006d/.

In the site-descriptive transport models, descriptions of conditions at the sites are given. In the Data Report and SR-Can assessment, evaluations are made for obtaining relevant input data on sorption characteristics. For example, a large variability in point values of sorption characteristics will be reduced when averaging along flow paths is made. It is the distribution of averaged values that serves as input for the radionuclide transport calculations.

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 water's flux 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.

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 ago, chemical reactions have transformed and affected the rock and its fracture system. During rock formation, water was released which also contained residual products that did not fit into the crystal lattice, such as chloride, sodium and calcium. This water is called juvenile, has always existed in the rock and usually contains large quantities of dissolved salts. If the salinity of the water exceeds 10 percent, i.e. 100 g/L TDS, it is called a brine /Frape and Fritz 1987/. Such water is stagnant due to its high density, which furthermore 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. Bruno has compiled reaction rates for different kinds of reactions /Bruno 1997/. The fastest are metal hydrolysis reactions, with half-lives ranging from microseconds to tenths of seconds. Then 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 haematite in water takes tens to tens of thousands of years, and dissolution of aluminium silicate takes tens of thousands to millions of years. There are, however, reactions between solid phase 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 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 significant in a time scale 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 the 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) occur and 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 a dried-up sea far back in time) 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 at one time by thick sediments which may also have contributed some brine component). In both cases, however, 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 constantly. 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 to 200°C, at repository depth have, in general, not occurred in the Fennoscandian shield since the Precambrian (i.e. in the last 570 million years), and in all cases they have never occurred after the Cretaceous (i.e. not in the last ≈ 65 million years). The effects in the rock of hydrothermal events are that material has been dissolved and cavities called druses have formed, whereas at other places large quantities of fracture-filling minerals have been deposited. Afterwards, these fracture systems 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 water-bearing fracture zones.

During the late Palaeozoic (400 to 250 million years ago), the overlaying sedimentary cover increased the bedrock temperature to 50–150°C during a period of at least hundred million years. Leaching of these sediments led to formation of saline waters and precipitation of fracture minerals like calcite (with very saline inclusions) and gypsum in the bedrock fractures. 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 as those that take place 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 only takes place by diffusion. There is no sharp borderline between water-bearing fractures and the rock matrix. So far, only modest attempts have been made to characterise the chemistry in the rock’s pore water. Studies in the URL 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 pore water and water in water-bearing fractures in the near-vicinity, essentially both being brackish /Smellie et al. 2003/. More recent studies at Laxemar indicate a similar pattern /Waber and Smellie 2005a/. In the upper bedrock, where the fracture frequency and transmissivity is higher than at depth, there is little difference between the chemistry of the matrix pore water and that of the formation groundwater in adjacent hydraulically active fractures. However, with increasing depth, and particularly where the bedrock is hydraulically tight, the matrix pore water is more saline than the formation groundwaters. Corresponding studies at Forsmark show a different trend, where the upper c 300 m of the bedrock is characterised by matrix pore water that is more dilute than the adjacent formation groundwaters. At larger depth, this trend is reversed and a pattern similar to the deep Laxemar samples is obtained /Waber and Smellie 2005b/.

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 ≈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 a glacier – exists in the minerals. 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-Can is also indicated in the table and further described in Section 5.5.7.

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

It is possible with the aid of thermodynamic calculation tools to determine which mineral alterations can be expected under different conditions. The accuracy of the data and knowledge of the reactions is sufficient. Knowledge of 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.

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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes. By changes in reaction types and rates.	Excavation/operation, Temperate, Permafrost	Process neglected; little expected impact.	Yes. By producing or consuming heat.	Excavation/operation, Temperate, Permafrost	Process neglected; little expected impact.
		Glaciation	Influence neglected; little significance compared with other influences.		Glaciation	Influence neglected; effect on temperature is negligible.
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, Permafrost	Process neglected; little expected impact.	No.	–	–
		Glaciation	Influence neglected; little significance compared with other influences.			
Gas 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.	–	See Section 5.10.	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.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Fracture geometry	Yes. Porosity affects mineral surfaces accessible to reactions.	Excavation/ operation, Temperate, Permafrost	Process neglected; little expected impact.	Yes. Weathering reaction may increase or decrease the porosity of the rock matrix.	All	Influence neglected; little expected impact.
		Glaciation	Porosity included in the modelling of the consumption of O_2 in infiltrating glacial meltwaters.			
Rock stresses	No. But indirectly by affecting matrix porosity.	–	–	No. But indirectly by changing porosity.	–	–
Matrix minerals	Yes.	Excavation/ operation, Temperate, Permafrost	Process neglected; little expected impact.	Yes.	Excavation/ operation, Temperate, Permafrost	Process neglected; little expected impact.
		Glaciation	Included in the modelling of the consumption in the rock matrix of O_2 infiltrating in glacial melt waters.		Glaciation	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 pore-water chemistry and matrix diffusion, but this is a very slow process.	–	–
Groundwater composition	Yes.	Excavation/ operation, Temperate, Permafrost	Although groundwater composition may be affected by grouting, etc, the propagation of these changes into the rock matrix has been neglected in SR-Can.	Yes.	Excavation/ operation, Temperate, Permafrost	Process neglected; little expected impact.
		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, Permafrost	Process neglected; little expected impact.	Yes. But negligible production of gaseous products by porewater-rock reactions	All	Neglected.
		Glaciation	Saturated conditions assumed.			

5.5.5 Time perspective

Very saline water, brine, will remain unchanged during the short (geologically speaking) period of time needed for a post-closure safety assessment of disposal of nuclear waste. 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 during glacial events the brines may migrate in the bedrock.

Chemical reactions that influence the composition of the water occur in a timeframe of thousands to hundreds of thousands of years. Producing a water with extremely high salinity (brine) requires much longer periods. The prevailing chemical groundwater composition is the result of many different ongoing reactions. Because they 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.

5.5.6 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 and from the various site investigations in Sweden and Finland. Geochemistry of crystalline basement brines has been documented from Canada, Russia and Fennoscandia. The oscillating behaviour of the brine/less saline interface during glacial events has been reported from the Sellafield site, UK /Bath et al. 2000/.

5.5.7 Handling in the safety assessment SR-Can

Excavation/operation, Temperate and Permafrost periods

The 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.

During the excavation/operation phase, when aerated waters could be expected to flow in fractures in the vicinity of the tunnels, or in the excavation damaged zone, chemical reactions are expected to take place only at the surfaces of fractures and not in the rock matrix. Therefore, mineral dissolution and transformation of the rock matrix is not modelled in SR-Can, except for periods of glaciation, see below.

Glaciation

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 in 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.

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 timespan relevant in disposal of spent nuclear fuel.

Model simplification uncertainties in SR-Can

Not relevant.

Input data and data uncertainties in SR-Can

Not relevant.

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 temperature changes and salt exclusion induced by freezing.

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 primary mineral phases to secondary ones. At the surface, this phenomenon is called chemical weathering, and the secondary mineral phases consist of different kinds of clay minerals. In crushed volumes (e.g. fault gouge), where both mechanical and chemical influences have occurred at different times since the rock was formed, there are large quantities of different secondary fracture-filling minerals. The sequence in which they have been formed can be revealed by careful mapping /Tullborg et al. 1991, Drake and Tullborg 2004, Sandström et al. 2004/. However, it is usually difficult to determine when and under what conditions this has taken place. Most fracture-filling minerals have originated under hydrothermal conditions (temperatures above 100°C and pressures well above 1 bar) far in the past. 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. Such precipitates are calcite, gypsum, pyrite, fluorite, amorphous silica and certain iron oxides. The existence of these mineral phases makes it possible to draw qualitative conclusions concerning the water chemistry that prevailed when the minerals were formed. 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, and causing precipitation of calcite on the fracture surfaces when 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 is the effect expected to be pronounced.

An idea can be obtained of the effects of fracture opening/closing by comparing the occurrence of healed and open calcite fractures near the ground surface and at greater depths. The proportion of healed fractures is estimated to be one-third at depths down to 100 m and two-thirds at depths greater than 100 m. This results from the combination of a faster hydraulic regime close to the ground surface and the infiltration of meteoric waters. There are, however, great local variations due to site-specific hydrological conditions.

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. This is important, since calcium destabilises colloidal particles at a concentration in excess of about 4 mg/L.

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 high values (1,290 and 399 mg/L for Mg and K, respectively) to below 150 mg/L for magnesium and 12 mg/L for potassium.

Influence on pH; The groundwater's pH normally lies 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 mineral in the rock's fracture system. The carbonate system quickly reaches a state of equilibrium and determines the water's pH, which will then lie around 8.5 /Stumm and Morgan 1981/. The total carbonate concentration often varies within the range 100 to 300 mg/L and seldom exceeds 600 mg/L. Extremely high carbonate concentrations can occur as a result of biological activity. Concentrations of 1,000 mg/L have been recorded on isolated occasions.

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 may be 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. The pH-buffering capacity which exists in the carbonate system in the groundwater, and which determines the pH, is however 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 /Chapman et al. 1993/, where a superficial groundwater with a pH of 3 was changed to 6–7 by reaction with feldspar /Nordstrom et al. 1992/.

Calcite minerals are a useful indicator of inflow of recently-infiltrated groundwater. In areas where carbon dioxide-rich groundwater has infiltrated the bedrock, calcite dissolution can be seen to have occurred down to a depth of about 100 m. The proportion of calcites in fracture-filling minerals in the water-bearing fractures can be estimated at 5 to 40 percent. 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 which prevail before the repository is built and which 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. The latter make 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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	**Time period**	**Handling of influence**	**Influence present?**	**Time period**	**Handling of influence**
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.
		Permafrost	Process neglected; of little significance to water composition and matrix porosity.			
		Glaciation	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	All	Neglected; effect on reaction rates and solubilities is negligible.	No.	–	–
Gas 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 chemistries/ reactions.	–	–	Yes. Geometry might be changed by the sealing or opening of some fractures.	Excavation/ operation, Temperate	Generic modelling that indicates that this influence is negligible.
					Permafrost Glaciation	Process neglected; little significance.
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.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	**Time period**	**Handling of influence**	**Influence present?**	**Time period**	**Handling of influence**
Fracture minerals	Yes. By aiding nucleation and growth of the same, or other precipitating fracture phases.	Excavation/operation, Temperate	Common fracture minerals (calcite, silica, etc) selected for generic equilibrium calculations.	Yes.	Excavation/operation, Temperate	Generic modelling.
		Permafrost	Process neglected; little significance.		Permafrost	Process neglected; little significance.
		Glaciation	Fracture minerals included in the modelling of consumption of oxygen in glacial meltwaters.		Glaciation	Effects of calcite dissolution and precipitation included in modelling of consumption of oxygen in glacial meltwaters.
Groundwater composition	Yes.	Excavation/operation,	Generic modelling of precipitation-dissolution of minerals.	Yes.	Excavation/operation,	Generic modelling of precipitation-dissolution of minerals.
		Temperate	Site-specific groundwater composition used as input to equilibrium calculations with common fracture minerals.		Temperate	Site-specific groundwater composition used as input to equilibrium calculations with common fracture minerals.
		Permafrost	Process neglected; little significance.		Permafrost	Process neglected; little significance.
		Glacial	Used as input to modelling of uptake of oxygen in glacial melt waters, including dissolution-precipitation of calcite, etc.		Glacial	Modelling of uptake of oxygen in glacial melt waters, including dissolution-precipitation of calcite, etc.
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.	Excavation/operation, Temperate,	Influence neglected; little significance.	No.	–	–
		Permafrost	Process neglected; little significance.			
		Glaciation	Neglected; saturated conditions assumed.			

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 Time perspective

The 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.

5.6.6 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 1997, Smellie 2002/.

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, conclusions about formation conditions can be obtained /Bath et al. 2000, Tullborg 2003/.

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/.

U contents and Uranium decay series analyses on groundwater and fracture minerals can indicate redox conditions over a time span of 1 Ma. Such analyses have bee carried out at Äspö and indicate changes from oxidising to reducing conditions within the upper 50 m of the bedrock /Tullborg et al. 2003/.

5.6.7 Handling in the safety assessment SR-Can

For the influence of co-precipitation on radionuclide transport, see Sections 5.4 and 6.1.

Excavation/operation and Temperate periods

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, pyrite and iron sulphide. The computer model PHREEQC is used for these calculations /Parkhurst and Appelo 1999/. The effects of precipitation-dissolution of minerals and grout are studied through generic calculations.

Permafrost

The effects of reactions between groundwaters and fracture-filling minerals under permafrost are not evaluated in SR-Can. The most distinctive processes under this period, in addition to freezing, may be salt exclusion and methane ice formation. This simplification will be evaluated in future safety assessments.

Glaciation

A qualitative analysis is made of the clogging of present-day flow paths and opening of others by precipitation and dissolution of calcite. This requires knowledge of the occurrence and variability of the calcites at the investigated sites.

Beneath a warm-based ice sheet, oxygenated water could possibly penetrate down to repository depth. Calculation of the reactions of oxygen during transport down into the rock is carried out. The groundwater modelling yields transport performance measures such as travel times and F-quotients, whereas the oxygen calculations answer the question of whether the oxygen is consumed during the descent of the water. Impacts of reactions with rock minerals is included, see Section 5.5.7.

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-Can

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. For the evaluation of oxygen consumption in meltwater during the glaciation period, neglecting the dissolution of some of the slowly reacting solids will give pessimistic (long) times for oxygen consumption.

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. However, changes in fracture properties, such as porosity, are not considered in SR-Can.

Input data and data uncertainties in SR-Can

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 their quantities and occurrence among 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 by oxidation of 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.

5.7 Microbial processes

5.7.1 Overview/general description

Microorganisms interact with their surroundings, and commonly have a significant effect on the geochemical record of the geosphere. Microbial processes could, therefore, significantly influence the functioning of any future high-level radioactive waste repository /Pedersen 2002/. The study of microbial processes in the laboratory can yield valuable information about possible microbial effects on such a repository. However, the effects suggested by laboratory studies must be tested in a repository-like environment for several reasons. First, at repository depth, hydrostatic pressure approaches 50 bars, a level that is very difficult to reproduce in the microbiology laboratory. Such high pressure influences the amount of gas that can be dissolved and may influence microbial processes. Second, the geochemical environment of deep groundwater, on which microbial life depends, is complex. Dissolved salts and trace elements, and in particular the redox chemistry and carbonate system, are characteristics that are very difficult to mimic in a research laboratory located at the ground surface level. Third, natural ecosystems, such as those in deep groundwater, comprise many different species in various community mixes /Pedersen 2001/; the surface-level laboratory, however, is best suited for studies of pure cultures. Therefore, the effect of processes arising from many contributing species in natural ecosystems cannot easily be investigated there.

One very clear example of the importance of understanding the microbial community structure can be extracted from Figure 5-2, illustrating the production of acetate from hydrogen and carbon dioxide by one group of microbes and the production of methane, sulphide or reduced iron by another group. This theoretical model is now supported by experimental efforts. Recent cultivation results from 450 m depth at Äspö have demonstrated how autotrophic acetogens produce acetate in cultivation test tubes using hydrogen and carbon dioxide as energy and carbon sources, respectively. Concomitantly, in the same tubes, sulphate-reducing bacteria produce sulphide and carbon dioxide, utilising acetate from the acetogens as a source of carbon and energy. This cultivation of two different types of bacteria in the same test tube is difficult to achieve and it demonstrates how important it is to study microbial community processes. As is discussed below, the importance of hydrogen as a base for microbial communities should not be underestimated. The extent and importance of hydrogen driven microbial community processes will be intensively studied in the Äspö URL.

The aforementioned limitations of surface-level investigations have motivated extensive microbiological investigations of deep Fennoscandian groundwaters over almost two decades. The work has resulted in a series of publications, as presented and reviewed elsewhere /Pedersen and Karlsson 1995, Pedersen 2000b, 2001, 2002/.

There are presently three specific microbial geosphere process areas identified that are of importance for safe repository function. They are:

- Microbial community effects on the chemical stability of deep groundwater environments.
- Bio-mobilisation of radionuclides.
- Bio-immobilisation of radionuclides.

Those processes are briefly introduced below.

Microbial effects on the chemical stability

Microbial energy metabolism requires a reduced electron and energy donor and an oxidised electron acceptor as summarised in Table 5-6. The energy donor can be an organic or an inorganic compound. The electron acceptor is generally an inorganic compound, with the exception of fermentation, where the electron donor and electron acceptor is the same organic compound. Electron donors and acceptors can be combined in redox couples according to the difference in free energy. Any redox couple that releases energy via a reaction is a possible source of energy for microbes /Pedersen and Karlsson 1995/. The result from microbial harvesting of energy from redox couples is an oxidised donor and a reduced acceptor. Important to notice here is that microbial metabolism generally lowers the redox potential in the environment. The hydrogeochemical analysis of data from the site investigations, and also from investigations in the Äspö HRL, suggests that microbes constitute a major redox control via their metabolic processes. It is hypothesised that deep groundwater would be more susceptible to oxidation without the redox buffer that microorganisms create. The fortunate thing here is that microbial processes will be steadily ongoing and they will not be exhausted as long as new energy is introduced. This energy is continuously supplied, mainly as energy rich gases such as H_2 and CH_4 from very deep crustal processes, at a rate limited by advection and diffusion processes /Apps and van de Kamp 1993/, and in this way made available for microbes /Amend and Teske 2005/.

Microorganisms can have an important influence on the chemical situation in groundwater /Pedersen 2001/. Especially, they may mediate reactions that stabilise the redox potential in groundwater at a low and, therefore, beneficial value for the repository. It is hypothesised that hydrogen from deep geological processes contributes to the redox stability of deep groundwater by microbial turnover of this gas /Pedersen 2000a/. Hydrogen, and possibly also carbon monoxide and methane, energy metabolism will generate secondary metabolites such as ferrous iron, sulphide and organic carbon, in particular acetate. These species contribute to a low redox potential and they will reduce oxygen if it is introduced.

The following microbial reactions are the most important with respect to geosphere processes. The reactions will occur as ordered with depth, with oxygen reactions occurring at high redox in surface groundwater and the last reactions appearing at depth where the redox potential is low, mainly as a result of microbial processes.

With oxygen

1. methane + oxygen → carbon dioxide + water (methanotrophic bacteria)
2. organic carbon + oxygen → carbon dioxide + water (many different microbes)
3. ferrous + oxygen → organic carbon + ferric iron (iron-oxidising bacteria)
4. sulphide+ oxygen → organic carbon + sulphate (sulphur-oxidising bacteria)

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	$\underline{C}O_2$	$\underline{Fe}^{2+}$	$\underline{Fe}^{3+}$	$\underline{Fe}^{3+}$	$\underline{Fe}^{2+}$
		$H_2\underline{S}$	$\underline{S}O_4^{2-}$	$\underline{S}O_4^{2-}$	$H_2\underline{S}$
		$\underline{C}H_4$	$\underline{C}O_2$	$\underline{S}^0$	$H_2\underline{S}$
		$\underline{C}O$	$\underline{C}O_2$	$\underline{U}O_2^{2+}$	$\underline{U}^{4+}$
		$\underline{H_2}$	$\underline{H_2}O$	$\underline{C}O_2$	$\underline{C}H_4$

Without oxygen

5. organic carbon + ferric iron/manganese(IV) → ferrous iron/manganese(II) + carbon dioxide (iron-reducing bacteria)
6. organic carbon + sulphate → sulphide + carbon dioxide (sulphate–reducing bacteria)
7. methane + sulphate → hydrogen + carbon dioxide + sulphide (anaerobic methane oxidation)
8. hydrogen + carbon dioxide → methane (autotrophic methanogens)
9. hydrogen + carbon dioxide → acetate (autotrophic acetogens)
10. acetate + sulphate/ferric iron/manganese(IV) → organic carbon + water (many different microbes)

A first case of special importance is the reduction of O_2 in microbial metabolism. Oxygen is the preferred electron acceptor by many microorganisms, because the free energy available in oxidation of an electron/energy donor is larger when oxygen is used than with other acceptors.

An early indication that microbial O_2 reduction may be of considerable proportions in granitic environments was published after a series of full scale atmospheric oxygen intrusion experiments into a 70 m deep vertical fracture zone at the Äspö HRL, Sweden /Banwart et al. 1996, Molinero et al. 2004b/. Later, the Monod equation for microbial kinetics was successfully used to model O_2 reduction during a series of field (also at Äspö HRL) and laboratory experiments (the REX project) aiming at the study of O_2 depletion in granitic media /Puigdomenech et al. 2001a/. The Monod equation (similar to the Michaelis-Menten kinetic used for microbial growth) describes the effect of the oxygen concentration on the oxygen reduction rate:

$$v = V_{\max} \frac{[O_2]}{K_S + [O_2]}$$

where v is the O_2 reduction velocity at a specific O_2 concentration, $V_{\max}$ is the maximum rate when the organism is O_2 saturated and K_S is the O_2 concentration when the O_2 reduction rate is ½ of the maximum. Over a wide range of O_2 concentrations tested in situ, the variation of v with respect to $[O_2]$ followed the empirical Monod equation, for details, see /Kotelnikova and Pedersen 1999/ and /Puigdomenech et al. 2001a/. These reports were later summarised in /Kotelnikova 2002/.

The most important conclusions from the Redox Zone and REX experiments were:

- Microbes play a substantial role in O_2 reduction in granitic media, and microbial processes imply a significantly enhanced reducing capacity in a repository environment, as they catalyse reactions that otherwise do not take place at low temperatures.
- When a surface water containing O_2 encounters the “stationary” groundwater system at depth, there is substantial increase in microbiological activity, resulting in O_2 depletion, transformation of organic material to CO_2 and formation of biofilms.
- The time scale for complete microbial oxygen reduction in typical fractures was estimated to be in the order of a few days.

Investigations of shallow Olkiluoto groundwater in May 2004 have demonstrated abundance of methanotrophic bacteria down to 25 m depth /Pedersen 2006/. It was found that oxygen concentrations decreased as a function of the presence of methane and methanotrophic bacteria, suggesting that these bacteria could constitute a barrier against intruding oxygen if sufficient methane is available.

A second case of importance is the fixation of carbon dioxide to organic molecules by autotrophic microorganisms under anaerobic conditions (Figure 5-2). The most important two groups are the autotrophic methanogens and the autotrophic acetogens. The methanogens

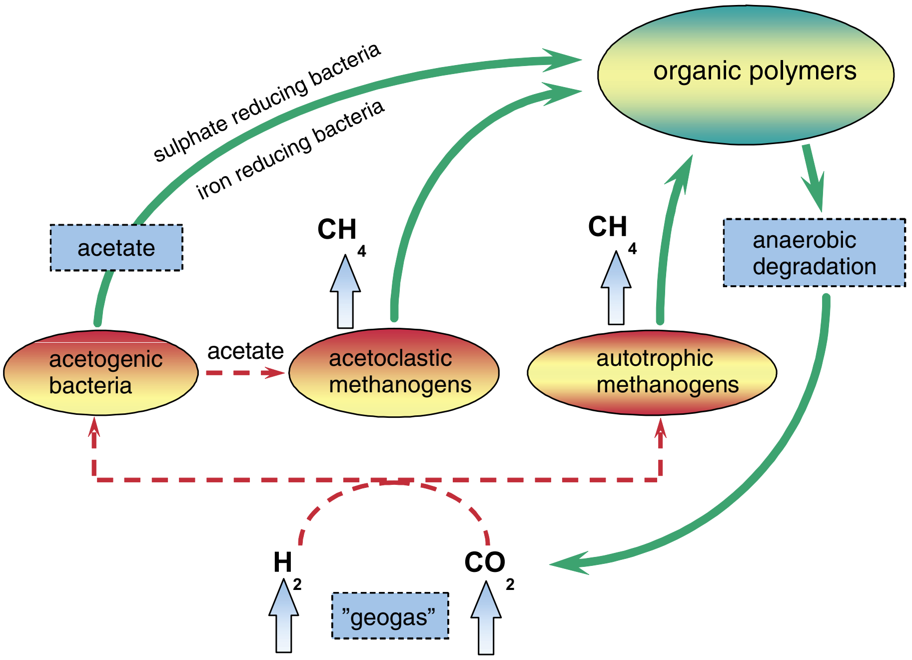

Figure 5-2. *The deep hydrogen-driven biosphere model, illustrated by the carbon cycle. At repository depth, the geosphere temperature and water availability conditions are such that subterranean microorganisms are capable of performing a life cycle that is independent of sun-driven ecosystems. Hydrogen and carbon dioxide from the deep crust of Earth can be used as energy and carbon sources. Phosphorus is available in minerals such as apatite, and nitrogen for proteins, nucleic acids, and other compounds can be obtained by nitrogen fixation, as nitrogen gas is present at adequate concentrations in many groundwaters.*

combine hydrogen and carbon dioxide to methane. Doing so, they produce biomass, methane and organic carbon. This is a renewable source of organic carbon to the geosphere which will guarantee that the oxygen reduction models described above will continue to operate for the lifetime of a repository.

Microbial processes that may influence radionuclide transport

Microbial processes can significantly alter the mobility of radionuclides in the environment. Table 5-7 summarises the microbial processes that can influence the speciation and thereby the migration behaviour of radionuclides. Microbial processes can have either immobilising or mobilising effects, depending on the type of process and the state of the microbes involved. Microbes in biofilms will, with the exception of those which produce complexing agents, be immobilising. Planktonic cells that biosorb or bioaccumulate radionuclides will have a mobilising effect on radionuclides. If the microbe is unable to move by its own mechanisms, it will transport radionuclides just like a large colloid. However, planktonic cells may have the ability to move in a desired direction as a response to various stimuli e.g. gradients of nutrients, light, oxygen or toxic substances. Doing so, they may override the prevailing groundwater flow direction and also the flow rate, as flow in deep fractures is generally very slow. However, the swim rate for microorganisms is also very slow at a repository depth scale. A normal microbe can swim about 1 mm per minute and really fast ones (e.g. *Bedellevibrio*) can move 5 mm per minute. It would take a normal microorganism about 24 h to move 1.5 m if it swims in a specific direction and about a year to reach the surface from a repository. However, as this is a gradient dependent movement, the microbe will only move as long as the gradient is established. Few gradients that microbes can sense are steep enough for more than a couple of cm. So, although microbial movement can be locally directed, it will, in a larger perspective, appear as random.

Table 5-7. Microbial processes can directly or indirectly influence retention of radionuclides in several ways. The most important variables in such processes are the state of attachment (i.e. whether the microbes are attached or unattached) and whether the microbes are metabolically active or dormant and inactive.

Microbial processes that influence radio-nuclide migration	Microbes in this process are in the following state(s):		This action of this microbial process on radionuclides is:		This process requires an active microbial energy-driven metabolism:	
	Planktonic	Biofilm	Direct	Indirect	Yes	No
Immobilisation processes						
Biosorption		X	X			X
Bioaccumulation		X	X		X	
Biotransformation	X	X	X		X	
Biomineralisation	X	X		X	X	
Metabolic redox reactions	X	X		X	X	
Mobilisation processes						
Biosorption	X		X			X
Bioaccumulation	X		X		X	
Production of complexing agents	X	X	X		X	

Microbial processes can act directly or indirectly in affecting radionuclide transport in the geosphere. Direct action involves contact between a microbe and the radionuclide, with a resulting change in radionuclide speciation. Indirect action is caused by changes in the environment generated by microbial metabolism, which in turn influence radionuclide behaviour. Finally, all microbial processes except biosorption require an active, energy-driven metabolism. Such energy is available at repository depth as reduced geo-gases, although the supply is limited by advection and diffusion. The modelling of microbial processes, therefore, must include a proper understanding of microbial energy turnover rates in deep rock aquifers as well as a careful consideration of the rates of supply of geo-gases.

Bio-immobilisation of radionuclides

Biosorption

The term biosorption (Table 5-7) is used to describe the metabolism-independent sorption of heavy metals and radionuclides to biomass, i.e. microbial cells. Biosorption can be summarised as the sorption and accumulation of trace elements to the surface of microbial cells. Both living and dead biomass are capable of biosorption, and the ligands involved in metal binding include carboxyl, amine, hydroxyl, phosphate, and sulphydryl reactive groups on the cell wall.

Microbe numbers as high as 10^{11} cells/m^2 have been reported in biofilms in Fennoscandian shield rock groundwater /Pedersen 2001/. Biofilm microorganisms commonly excrete extra-cellular material supporting attachment, and this material also creates the three-dimensional shape of a growing biofilm. As this extra-cellular material is organic in nature, it adds a biosorption capacity to that of the cell's surfaces. In conclusion, biosorption to attached microbes in biofilms can have an immobilising effect on radionuclides.

Very few in situ experimental data exist regarding the importance of biofilm biosorption processes as a contribution to geosphere retention phenomena in the context of the safety assessment of radioactive waste disposal. In response to this lack, ongoing experiments are attempting to elucidate these processes. In situ experiments on radionuclide retention on microbial biofilms and rock show some unexpected results for ^{60}Co(II), ^{147}Pm(III), ^{241}Am(III), ^{234}Th(IV), ^{237}Np(V) and ^{99}Mo(VI) /Anderson et al. 2005ab/. Partial screening of the rock surface due to biofilm growth was evident, with a decrease in rock adsorption capacity, in particular, for Co(II). The biofilm induced increased sorption of promethium only. Anaerobic biofilms and rock surfaces share similar adsorption capacities, but probably have dissimilar complex stability due to the surface functional groups available and competition for those groups. Several factors, such as groundwater composition and chemical properties of the radionuclide species, may limit the effectiveness of biofilm surfaces as a sorbent. In addition, there may be a competition between calcium and magnesium and divalent cationic radionuclides. Microbial cells have high affinity for calcium and magnesium ions in their cell membranes. The possible suppression of adsorption of divalent cationic radionuclides by biofilms should be further studied experimentally and, if possible, accounted for in future performance safety assessment models.

Bioaccumulation and biomineralisation

A large group of microbes catalyse the formation of iron oxides from dissolved ferrous iron in groundwater that reaches an oxidising environment /Ferris et al. 1999, 2000/. Such biological iron oxides (BIOS) will have a retardation effect on many radionuclides. Typically, those microbes form stalks and sheaths that increase the volume of the iron oxides yielding not densely packed inorganic oxides but rather a fluffy, rust-like material with a water content of up to 99%. The microbes contribute to the exposure of a large oxide area to trace elements flowing past in the groundwater; also, the organic biological material has a strong retention capacity of its own. The retention effect of BIOS (bioaccumulation and mineralisation, Table 5-7) has been studied /Anderson and Pedersen 2003/. It was found that BIOS has a significant immobilising effect on various trace elements.

Bio-mobilisation of radionuclides

Microbes need metals for their metabolism, as do multicellular living organisms, and both bacteria and microscopic fungi share this need. Some of these metals are often available only in small quantities or, as with iron in surface waters, are not bio-available at all due to low solubility under aerobic conditions. Therefore, microbes produce various kinds of chelating compounds to increase the bioavailability of essential elements needed for metabolism, called siderophores. These ligands are not always highly specific, and several of them will also mobilise other elements such as heavy metals and radionuclides. As for artificial ligands, such as EDTA, the bonding with trivalent metal cations, e.g. Fe(III), is orders of magnitude stronger than the bonding with monovalent and divalent cations like Na^+ and Ca^{2+} that are abundant in natural waters. In the process of capturing the metal−ligand complex, microbes sort toxic metals from essential ones and expel the toxic elements back to the environment. The potential for the mobilisation of radionuclides from repository environments by bacterially produced ligands is unknown; therefore it warrants further exploration. This process has been investigated in the laboratory using microorganisms isolated from the deep groundwaters of the Äspö HRL. It was found that the studied bacteria produced at least 4 potent complexing agents /Arlinger et al. 2004/. Ongoing experiments have also demonstrated a mobilisation effect on americium by chelating agents from bacteria grown under anaerobic conditions /Arlinger et al. 2004/. In situ experiments will address the possible influence of these ligands if present under natural undisturbed conditions.

Fungi have the ability to produce large amounts of complexing agents, for example, via fermentation processes. The presence of fungi in deep groundwaters has been noted in earlier work: a detailed survey of fungi found in Äspö groundwaters was reported in /Ekendahl et al. 2003/.

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 a metal atom for a hydrogen atom of a methyl group molecule. 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. 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/. The radionuclide is not only mobilised, but also its 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).

5.7.2 Dependencies between process and geosphere variables

Table 5-8 shows how microbial processes are influenced by and influence all geosphere variables. The handling in SR-Can is also indicated in the table and further described in Section 5.7.7.

Table 5-8. Direct dependencies between microbial processes and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes. Most microbes have an ideal temperature range in which they thrive. Maximum temperature for life is well above 100°C.	Excavation/ operation, Temperate	Influence neglected; little significance compared with other influences.	No.	–	–
		Permafrost	Process not handled in SR-Can.			
		Glaciation	Process not handled.			
Groundwater flow	No. But indirectly through transport of nutrients which is a requirement for microbial metabolism. Microbial activity correlates positively with flow rate.	–	–	No. But indirectly; microbial activity may over time contribute to the generation of fracture minerals that eventually seal a fracture.	–	–
Groundwater pressure	Yes Most microbes have an ideal pressure range in which they thrive. This range is commonly very large. Indirectly by affecting solubility of gases (see row groundwater composition below).	Excavation/ operation, Temperate	Influence neglected; little significance compared with other influences.	No.	–	–
		Permafrost	Process not handled in SR-Can.			
		Glaciation	Process not handled in SR-Can.			
Gas flow	No. But transport of energy for living is a requirement for microbial metabolism. This energy may be carried by a gas phase, e.g. as methane or hydrogen.	–	–	No. But indirectly by changes in fracture geometry (aperture).	–	–
Repository geometry	No.	–	–	No.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Fracture geometry	No. But indirectly since transport of nutrients is a requirement for microbial metabolism. Non-conductive or isolated fractures will not be able to supply nutrients.	–	–	No	–	–
Rock stresses	No.	–	–	No.	–	–
Matrix minerals	No. Microbes are not expected in the rock matrix. However, they may access trace elements in minerals via complexing agents.	–	–	No. But indirectly through diffusion of microbial metabolic products into the matrix affecting weathering reactions. This process is of negligible importance.	–	–
Fracture minerals	Yes. Microbes attach themselves in biofilms at the surface of fracture filling minerals. These minerals provide nutrients by dissolution reactions.	Excavation/operation, Temperate	Biofilms on fracture surfaces not considered.	No. But indirectly through changes in water composition. Metabolic products, e.g. CO_2, influence mineral dissolution. Some microbial metabolism products, e.g. sulphide, make new minerals.	–	–
		Permafrost	Process not handled in SR-Can.			
		Glaciation	Process not handled in SR-Can.			
Groundwater composition	Yes. Groundwater provides nutrients for microbial metabolism.	Excavation/operation, Temperate	Influence not considered.	Yes. Metabolic products will affect ground-water, e.g. by production of CO_2 and acetate, and perhaps redox properties, e.g. by sulphate reduction to sulphide.	Excavation/operation, Temperate	Evaluation of microbial activity and microbial metabolism products.
		Permafrost	Process not handled in SR-Can.		Permafrost	Process not handled in SR-Can.
		Glaciation	Process not handled in SR-Can.		Glaciation	Process not handled in SR-Can.
Gas composition	No. However, energy is required for microbial metabolism. This energy may be present in a gas phase, e.g. methane. The gas phase (if present) will influence groundwater composition, see interaction above.	–	–	No. But indirectly microbial metabolic products may, e.g. produce CO_2 or methane, and this could affect the composition of a gas phase if present.	–	–
Structural and stray materials	Yes. Nutrients are required for microbial metabolism. These nutrients may be present in the stray materials.	Excavation/operation, Temperate,	Evaluation of degradation of organic materials.	Yes. Microbes may use stray organic material for their metabolism. Microbial metabolic products may affect the corrosion and decomposition of structural materials (steel and cement).	Excavation/operation, Temperate,	Evaluation of degradation of organic materials
		Permafrost	Process not handled in SR-Can.		Permafrost	Process not handled in SR-Can.
		Glaciation	Process not handled in SR-Can.		Glaciation	Process not handled in SR-Can.
Saturation	Yes. Some microbes thrive at the interface between a gas and an aqueous phase.	Excavation/operation, Temperate,	Influence not considered.	No. Negligible production of gases by microbes.	–	–
		Permafrost	Process not handled in SR-Can.			
		Glaciation	Process not handled in SR-Can.			

5.7.3 Boundary conditions

There are no particular conditions at the geosphere boundaries for the microbial processes. The relevant conditions in order to treat the microbial processes quantitatively are the concentrations, in the different parts of the system being modelled, of nutrients and of electron acceptors and donors. For example, the concentrations of solutes in the groundwater flowing over the flow-wetted surface area where a biofilm has grown.

5.7.4 Model studies/experimental studies

Besides the above-mentioned studies, great efforts have been made to demonstrate – both by means of models and experimentally – that reducing conditions exist at repository depth. Presently, in situ experiments are ongoing at the Äspö HRL, to explore microbial redox processes /Pedersen 2005/. These experiments should elucidate in more detail if microbial production of complexing agents is of any quantitative importance for safety. The effect from biofilms on rock sorption and matrix diffusion is also being addressed.

The microbial contribution to oxygen consumption in fractures has been evaluated by /Sidborn 2003/. In addition, coupled groundwater flow and biogeochemical reactive transport models have been developed recently and applied to long-term, large-scale experiments such as the Äspö Redox Zone /Samper et al. 2003, Molinero et al. 2004a/. The reactive transport model accounts for organic matter fermentation and respiration of dissolved organic carbon through the reduction of ferric minerals available in the fracture zones. Model results confirm that even in absence of oxygen, oxidation of DOC is catalysed by iron-reducing bacteria, thus providing additional redox buffering to the groundwater system /Molinero et al. 2004a/.

5.7.5 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, but as "low pH" cement materials will be used, this effect will be limited.

Changes in groundwater flow and chemistry induced by climate related changes, e.g. by permafrost, ice sheets and shore line 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 diffusing 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.

5.7.6 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 /Haveman and Pedersen 2002/. The results confirm 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.

5.7.7 Handling in the safety assessment SR-Can

The handling of microbial processes in radionuclide transport is discussed in Section 5.4.

Excavation/operation and Temperate periods

Mass balance calculations are made to show how different kinds of residual organic materials remaining in the repository will react. It is assumed that all organic matter will be able to serve as nutrients for microbes. During this 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. An estimate is made of how large these quantities could be, and what consequences this process may have.

The availability of hydrogen will be a primary control on microbial activity in the long term. During the initial periods, an increased microbial activity must be expected until all residual organic matter has been consumed, whereas the subsequent microbial activity will be controlled by the supply of hydrogen. In the long run, all oxygen and some of the iron(III), sulphate and carbon dioxide will be reduced.

Permafrost

The consequences of microbial processes under permafrost are not analysed in SR-Can, as the characteristic processes under this period, in addition to freezing, are salt exclusion and methane ice formation. This simplification will be evaluated in future safety assessments.

Glaciation

Periods of glaciation 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, 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, during the Matrix experiments at Äspö, it was found 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.

In future safety assessments it will be attempted to analyse coupled groundwater flow and multi-component solute transport with hydrochemical and microbial processes for a glaciation scenario in which melting waters are rich in oxygen and contain no organic matter.

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. Some details need further exploration:

- The effect of microbial biofilms on the retardation of divalent cations by excluding them from rock surfaces is a recently discovered process that needs to be accounted for in safety assessments, and further explored.
- The possible production of complexing agents by microbes is not yet fully understood.
- 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 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.

Model simplification uncertainties in SR-Can

Modelling of microbial activities generally makes use of the Monod equation described above. The computed rates are generally fast as compared with the time scales of advection combined with matrix diffusion and reactions with rock matrix minerals /Sidborn 2003/. 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 introduced simplifications, 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 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 has been consumed, the subsequent microbial activity will be controlled by the supply of hydrogen and methane. In the long run, some of the sulphate will perhaps 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. The consequences of such a process are being evaluated, and will be included in future safety assessments.

Input data and data uncertainties in Sr-Can

Great variability exists in where and to what extent the different microbial processes occur. However, bacterial reduction of oxygen in the shallow groundwater occurs widely.

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. 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 which cannot be fully representative of repository conditions. Results of current in situ microbe investigations, as well as model calibration based on field experimental data /Molinero et al. 2004b/ 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.

5.8 Degradation of grout

5.8.1 Overview/general description

Depending on the fracturing of the rock close to the galleries and deposition tunnels, rock bolts, shotcrete and grouting might be used to: a) reinforce the rock to ensure safe working conditions; b) to 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. These inorganic materials are not chemically stable in a deep repository and will eventually decompose and affect the groundwater composition.

Rock bolts are considered to be part of the backfill in the system components definition of SR-Can. Nevertheless, they are discussed here as their degradation might affect the chemistry of the adjacent geosphere. Iron and steel will corrode with hydrogen formation: $3Fe + 4H_2O \rightarrow Fe_3O_4(s) + 4H_2$. Hence, the main resulting corrosion product is magnetite, and the corrosion process has no appreciable effects on the groundwater chemistry.

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 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, alumino-ferrite, 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, although the actual recipe /SKB 2004e/ will probably be optimised before the repository construction and during the relatively long period of repository operation. 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 which 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. The dissolution of highly soluble calcium hydroxide (portlandite) and 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/. Perhaps the most relevant features of C-S-H solubility concern 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/. Recent studies /Chen et al. 2004/ suggest that C-S-H solids are present under different metastable phases which are susceptible to transform (recrystallise) into one another in the long term.

Simultaneously with the dissolution of calcium silicate hydrates, the rest of mineral phases are also involved in the cement leaching phenomena. AFm dissolution releases $Al(OH)_4^-$ which will also out-diffuse and 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 salts (i.e. aluminium and calcium chlorides).

Sulphuric, nitric and organic acid-producing bacteria may degrade concrete /Diercks et al. 1991, Rogers and Hamilton 1993/. 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, which the deep repository is deficient in, compared with, for instance, the SFR repository. 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.

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. 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 5-9 shows how the process is influenced by and influences all geosphere variables. The handling in SR-Can is also indicated in the table and further described in Section 5.8.7.

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.

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/. 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/.

Table 5-9. Direct dependencies between the process "Degradation of grout" and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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.	–	–
		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.			
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; assumptions made regarding grout properties in different applications.	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.	–	–
		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.			

Variable	Variable influence on process			Process influence on variable		
	Influence present?	**Time period**	**Handling of influence**	**Influence present?**	**Time period**	**Handling of influence**
Gas flow	Yes. Large gas flows may affect the mechanical stability of the grouting.	All	Not specifically addressed; assumptions made regarding grout properties in different applications.	Yes. Degraded cement grout might be more permeable for a gas phase flow.	All	See Section 3.2.
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.
		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.		Permafrost Glaciation	Process not handled.
Rock stresses	Yes. Rock stress might physically break the grouting.	All	Not specifically addressed; assumptions made regarding grout properties in different applications.	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.
		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.		Permafrost Glaciation	Process not specifically addressed; extrapolation of results fromTemperate period.
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.
		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.
Saturation	Yes. Cement degradation is negligible in unsaturated rock.	Excavation/ operation Temperate	Saturated conditions assumed.	No.	–	–
		Permafrost Glaciation	Process not specifically addressed; extrapolation of results from Temperate period.			

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/.

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/.

Experience from the grouting performed during the construction of the Äspö tunnel shows that large quantities of standard cement mortar cause small and short-lived changes in the pH of the groundwater /Rhén et al. 1997/.

The consequences of cement grout degradation on the surrounding rock may be inferred from a field experiment at the Grimsel Test Site, where hyper-alkaline waters (pH = 13.4) were forced at a constant rate to flow in a fracture between two boreholes /Mäder et al. 2004/. The data showed a decrease in hydraulic transmissivity due to the formation of C-S-H phases in the fracture. As a consequence, increasing pressures had to be applied to the injection borehole, and the fluid flow in the fracture had to converge into the smaller porosity path. This resulted in increasingly shorter break-through times and higher breakthrough concentrations for non-reactive tracers.

5.8.5 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. According to some model studies /Höglund 2001/ the time perspective for grout degradation can be estimated as 10,000 years.

5.8.6 Natural analogues/observations in nature

Silicate minerals in granitic bedrock react with hydroxide ions, which may derive from cement. The silicate minerals dissolve as a consequence of hydrolysis reactions, after which secondary reaction products are precipitated. The course of the reaction has been studied at the hyperalkaline springs in Maqarin, Jordan /Smellie 1998/. The reaction rate is unknown, but it is estimated that the reaction can reduce the pH from about 13 to the range 10–11 and that it is presumably an extremely thin layer of minerals that reacts.

5.8.7 Handling in the safety assessment SR-Can

This process does not need any detailed modelling in SR-Can in view of the fact that the quantities are relatively small and that "low-pH" cement grouting will be used. However, 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.

5.8.8 Uncertainties

Uncertainties in mechanistic understanding

A main uncertainty is related to the complex solubility behaviour of C-S-H phases, which has been oversimplified in previous models of cement degradation. Other uncertainties are associated with the long-term evolution of the pore network and the diffusivity in the cement paste. The diffusivity depends strongly on the porosity values, and the coupling between the dissolution processes and the resulting microstructural changes are not fully understood.

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 analyses.

Model simplification uncertainties in SR-Can

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 is a simplification of the C-S-H phases that precipitate in reality.

Mechanical stability has little effect on grout function, although fracturing, e.g. as a consequence of seismic activity, could accelerate grout degradation.

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. Changes in fracture porosity are however not considered in SR-Can.

Input data and data uncertainties in SR-Can

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.

5.9 Colloid formation and transport

5.9.1 Overview/general description

Colloids are small particles, in the size range of 1–1,000 nm. They can stay in suspension for very long times because of surface charge effects and low gravitational settling velocity. For the smallest colloids, Brownian motion may prevail over gravitational forces, in which case the colloids will stay in suspension for ever. The border line between dissolved species and colloids at the lower size limit is diffuse, but particles smaller than 1 nm may be considered as dissolved molecules. In groundwater, colloids can form by erosion of rock material and sedimented mineral oxides, precipitation of mineral oxides and degradation of organic material. Also bacteria can be present, which comprise a special group of colloids, and are often larger than 200 nm. Coagulation followed by sedimentation removes colloids from the groundwater, as well as filtration and precipitation of colloids on mineral surfaces. Aggregation is influenced by particle size and groundwater composition, mainly pH and the concentration of cations.

In dilute groundwater, natural colloids are stable and can therefore be present in higher concentrations in comparison with saline waters, where the colloids are not stable. When the concentration of Ca^{2+} exceeded 10^{-4} M or Na^{+} 10^{-2} M, the natural colloid concentration was found to be less than 10^{-4} g/L (for colloids > 100 nm) in groundwater at the Grimsel test site /Degueldre et al. 1996/. Bentonite colloids follow the same type of behaviour and are particularly unstable in the presence of divalent ions such as Ca^{2+} and Mg^{2+} /Degueldre et al. 1996/.

In contrast, the slightest admixture of atmospheric oxygen in a reducing groundwater gives rise to extensive colloid formation. Immediately after closure of the repository, iron(II) dissolved in groundwater will react with entrapped air, mostly in the buffer and backfill, but also small amounts in the excavation damaged zone (EDZ) and in the rock matrix and around the tunnel walls. This chemical reaction will produce colloidal iron(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 concentration of colloids could theoretically increase in deep groundwaters in connection with the melting of a glacier following an ice age, because the recharging melt waters would have a low content of salt. In addition, glacier melt waters might contain dissolved oxygen, which could induce the oxidation of Fe(II) in near-surface waters, resulting in colloidal Fe(III) oxyhydroxides. However, studies show that low concentrations of colloids may persist even then, since the expected dilution does not result in the low calcium concentrations that are required for stable colloids to form /Laaksoharju et al. 1995b/.

Colloid migration in granite fractures is governed by the ability of the colloids to stay in solution. Advective transport is clearly dominating, since diffusion of colloids in the rock matrix is extremely slow. Sedimentation and filtration will remove colloids from the water. The sedimentation process is affected by the particle size and density and the gravitational settling is counteracted by Brownian motion. Sedimentation is favoured by aggregation. A decrease in the colloid surface charge by e.g. a decrease in pH, or a decrease in the double layer around the colloids by the addition of salt, gives aggregation followed by sedimentation.

Colloids can be transported 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/.

Filtration effects, which refer to immobilisation of colloids from the water, can be divided into straining and physical-chemical filtration /Moridis et al. 2003/. Straining filtration occurs when the colloids are larger than the pore diameter or fracture aperture, or when the colloids are larger than the thickness of the absorbed water film coating the grains of the rock. Physical-chemical filtration occurs when colloids come in contact with the pore walls or by fixation onto the fracture wall. Sedimentation and diffusion as well as hydrodynamic effects will give contact between the colloids and the fracture wall /Moridis et al. 2003/. The colloids will fixate on retention sites by, for example, friction forces, van der Waals forces, electrical and chemical forces. The filtration effect for colloids in a granite fracture is not known, but will be studied in a granitic fracture at Äspö using latex colloids.

Radionuclides can sorb (adhere) to colloidal particles and be transported with them. It is therefore important to estimate to what extent such particles can occur or be formed in the groundwater and for what time periods these particles can be stable.

Sorbed radionuclides could, in principle, be transported more or less unretarded with the velocity of the water if they adhere to colloidal particles in the groundwater /Laaksoharju et al. 1995b/. If the uptake of radionuclides on colloidal particles is reversible, this process will be manifested as a reduction of the K_d value, where the reduction is inversely proportional to the concentration of colloids and the sorption tendency on the colloids. This reduction is, however, negligible given the maximum colloid concentrations in Swedish rock at undisturbed conditions /Allard et al. 1991/.

If, on the other hand, the radionuclide should adhere irreversibly, the situation may be different. In this case, the radionuclide will be transported with the particle and, at worst, not be delayed at all by either sorption on fracture walls or by matrix diffusion in the rock. However, calculations show that the consequences are of no importance for safety in this case as well, due to the fact that the natural concentration of colloids is so low. The evaluation is summarised in /Allard et al. 1991/.

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. If present in large concentrations, the hydrolysis products contain several metal ions (polynuclear) and by aggregation they can form colloidal particles. In the case of plutonium, the formation of colloids is practically irreversible. However, the concentration levels needed for the formation of actinide colloids will never be reached in the geosphere.

In summary, it can be said that radionuclides in the groundwater can occur sorbed on colloids, and that the possibility that a small fraction will be bound irreversibly to mobile natural colloidal particles cannot be entirely excluded. However, as long as dose calculations are dominated by weakly or non-sorbing radionuclides, the overall consequence of colloid enhanced transport for the safety of the repository is negligible.

5.9.2 Dependencies between process and geosphere variables

Table 5-10 shows how colloid formation and transport is influenced by and influences all geosphere variables. The handling in SR-Can is also indicated in the table and further described in Section 5.9.7.

Table 5-10. Direct dependencies between the process "Colloid formation and transport" and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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. Furthermore, although the flow will not affect colloids in itself, colloids might form when groundwaters mix and by erosion.	All	Process neglected; insignificant impact on geochemical conditions.	No.	–	–
Groundwater pressure	No	–	–	No.	–	–
Gas flow	No. Colloids do not form in a gas phase. Even though it cannot be excluded that colloids are transported by 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 sub-sequent 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.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Repository geometry	No.	–	–	No.	–	–
Fracture geometry	No. Although the geometry of fractures will not affect colloids in itself, colloids might form when groundwaters mix.	–	–	No.	–	–
Rock stresses	No.	–	–	No.	–	–
Matrix minerals	No.			No.		
Fracture minerals	Yes. Colloids might form by resuspension of e.g. clays in very diluted waters.	Excavation/ operation, Temperate	Process neglected; insignificant impact on geochemical conditions.	Yes. Suspended colloids might sediment into fracture walls, e.g. when groundwaters mix.	Excavation/ operation, Temperate	Process neglected; insignificant impact on geochemical conditions.
		Permafrost Glaciation	Influence neglected; little significance See also Section 6.1 Radionuclide transport and Buffer erosion in Buffer and Backfill Process Report /SKB 2006g/.		Permafrost Glaciation	Influence neglected; little significance See also Section 6.1 Radionuclide transport and Buffer erosion in Buffer and Backfill Process Report /SKB 2006g/.
Groundwater composition	Yes. Concentration of dissolved salt affects the stability of colloids. Colloids might form by precipitation from oversaturated solutions.	Excavation/ operation, Temperate	Process neglected; insignificant impact on geochemical conditions.	Yes. Precipitation of colloids from oversaturated solutions will change the composition of the groundwater.	Excavation/ operation, Temperate	Process neglected; insignificant impact on geochemical conditions.
		Permafrost Glaciation	See Section 6.1 Radionuclide transport and Buffer erosion in Buffer and Backfill Process Report /SKB 2006g/.		Permafrost Glaciation	See Section 6.1 Radionuclide transport and Buffer erosion in Buffer and Backfill Process Report /SKB 2006g/.
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	Process neglected; insignificant impact on geochemical conditions.	No.	–	–
		Permafrost Glaciation	Influence neglected; little significance. See also Section 6.1 Radionuclide transport and Buffer erosion in Buffer and Backfill Process Report /SKB 2006g/			
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, Temperate	Process neglected; insignificant impact on geochemical conditions.	No.	–	–
		Permafrost Glaciation	Influence neglected; little significance. See also Section 6.1 Radionuclide transport and Buffer erosion in Buffer and Backfill Process Report /SKB 2006g/.			

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 0.05 mg/L has been 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 is pessimistically high, especially when considering the background colloid concentration measurements performed in Grimsel, /Degueldre et al. 1996/, where the natural colloid concentration was found to be less than 10^{-4} g/L (for colloids > 100 nm) in groundwater containing more than 10^{-4} M Ca^{2+} or Na^{+} 10^{-2} M. Also when considering that the colloid content in different Äspö groundwaters was measured to be less than 300 ppb, and at repository depth less than 50 ppb /Laaksoharju 2003/, 0.05 mg/L seems to be very high.

Laboratory tests confirm that radionuclides can sorb on colloids and that the sorption on mineral colloids is largely reversible. The strength of the sorption is roughly equivalent to the measured K_d for the corresponding minerals and radionuclides /Christiansen-Sätmark 1995/.

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. 2003/. 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. 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.

5.9.5 Time perspective

Extensive colloid formation can be expected in conjunction with closure of the repository, when mixing of oxidising and reducing water 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 area. 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).

5.9.6 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.

5.9.7 Handling in the safety assessment SR-Can

Colloids have negligible impact on the geochemical conditions of the geosphere.

Excavation/operation and Temperate periods

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/. 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. For further discussion, see Section 6.1.

Permafrost

The consequences of colloids under permafrost are not analysed in SR-Can, as the characteristic processes under this period, in addition to freezing, are salt exclusion and methane ice formation. This simplification will be evaluated in future safety assessments.

Glaciation

Melt waters from an inland ice sheet may have low concentrations of dissolved salts, and could stabilise colloids and erode the bentonite buffer. Analyses of buffer erosion and colloid release will be undertaken if the total concentration of divalent ions in the groundwater is 1 mM or less. This is further described in the process report for Buffer and Backfill /SKB 2006g/.

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-Can

See Section 6.1.8.

Input data and data uncertainties in SR-Can

See Section 6.1.8.

5.10 Formation/dissolution/reaction of gaseous species

5.10.1 Overview/general description

As indicated in Section 3.2, 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 chemical and dissolution processes in which the gases found in the geosphere may be involved.

Formation of gaseous species

There are a number of sources which may give rise to the presence of gases in the geosphere, namely:

- the existence of natural gases in solution in the groundwater,
- the generation of gases in the repository, principally from the anoxic corrosion of iron and steel,
- air trapped in the repository and desaturated rock at repository closure.

The type of natural gases likely to be present in solution in groundwater at a repository site is discussed in Section 3.2.1. There are different hypotheses concerning the origin of these gases. The concentrations of some gases can be explained by the fact that infiltrating groundwater has been saturated with respect to the gas components present in the air. In deep groundwater, the oxygen has normally been consumed by reactions, whereas the other components of atmospheric gases are found in the same proportion as in air. Very high concentrations of hydrogen and methane encountered in some locations are assumed to derive from molecular diffusion or groundwater advection from the interior of the earth, or to be the result of extensive bacterial activity /Pedersen 1997/. Noble gases (helium, neon, argon, etc.) which are present can be important as geodynamic tracers, providing information about the degassing history of the mantle, about the formation of the atmosphere, and about mixing relationships between different mantle components. However, there their concentrations are not likely to be significant for repository performance.

The formation of methane hydrates during colder climate conditions is discussed in Section 5.11. The decomposition of these methane hydrates as temperature rises might be a large source of methane.

Dissolution of gases

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, see also Section 3.2.1. There is intrinsic variation in the solubilities of the different gases, but for all of them the solubility depends on both the gas pressure and temperature. Gas solubility is, to a good approximation, directly proportional to the gas pressure (Henry's Law), and also decreases with an increase in temperature. If several gases together contribute to the total pressure, the solubility of each gas is proportional to its partial pressure, that is, the pressure the gas would exert if the mass of the gas present in a given volume was present on its own in that volume. 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 radioactive waste 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. Solubility normally reduces with an increase in ionic strength (the salting-out effect), although this effect is generally smaller than that of temperature and total pressure.

The concentration of gases in groundwaters varies between sites and depending on the gas analysed (Figure 5-3). Nitrogen generally dominates. In Olkiluoto, the methane concentration dominates at depth. The volume of dissolved gases ranges from some 10–20 mL per litre of groundwater at depths below 100 m up to 1,100 mL as observed at 900 m depth in Olkiluoto. At repository depth, the volumes of dissolved gas analysed at the Swedish and Finnish investigation sites and at Äspö are below 100 mL, except for Olkiluoto where the volume averages at about 500 mL.

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 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:

$$p_g = \sum_i p_{gi}$$

Participation of gases in chemical processes

Depending on their reactivity, gases may participate in (and be produced by) chemical reactions and microbial processes in the geosphere. These processes are natural long-term processes. In near-surface waters, dissolved oxygen of atmospheric origin may be present. However, oxygen is reactive, in particular oxidising dissolved Fe(II) and reacting with Fe(II) minerals, and

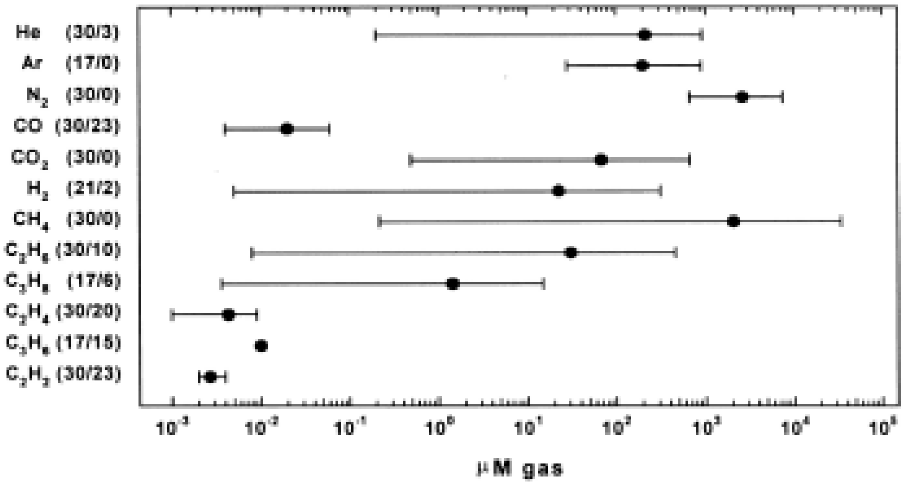

Figure 5-3. *The concentration of gas observed in Swedish and Finnish groundwaters. The figure shows the mean composition of the chemical species measured (filled circles); the bar gives the range. The number in parenthesis for each gas species are the total number of observations followed by the number of observations below detection limit. (Figure from /Pedersen 2002/).*

providing the preferred electron acceptor for many microbes (see Section 5.7). This reactivity quickly removes the oxygen from the groundwater and so it is not usually present by the time the groundwater has infiltrated to greater depths, with the result that deep groundwater usually has reducing chemistry. During repository operations, there will be some desaturation of rock around the repository and in the rock 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. Methane and hydrogen may be depleted from groundwaters if microbes use these molecules as electron donors[6].

Dissolved carbon dioxide, CO_2, is important to natural mineralogical processes that occur in the geosphere. It dissolves 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 reactions of fracture filling carbonates (calcite),

$$H_2CO_3(aq) + Ca^{2+} \leftrightarrow CaCO_3(s) + 2H^+$$

the weathering of minerals in the rock matrix (here exemplified by the weathering reaction of Ca-feldspar, anorthite, into kaolinite):

$$CaAl_2Si_2O_8(s) + 2H_2CO_3(aq) + H_2O \leftrightarrow Al_2Si_2O_5(OH)_4(s) + 2HCO_3^- + Ca^{2+}$$

and microbial processes (see also Section 5.7):

organic carbon + oxygen → carbon dioxide + water (many different microbes)

All these reactions affect the concentration of carbon dioxide present. Although the presence of dissolved carbon dioxide in groundwaters is important for geological processes, and the possible effect of its presence needs to be considered in assessing corrosion rates, there is not expected to be any carbon dioxide generated in the repository and, thus, there is nothing apart from its possible effect on corrosion rates that will make the presence of dissolved carbon dioxide significant for repository safety. The same is true for other dissolved gases. 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.

The main gas produced in the repository, hydrogen, may provide a substrate for microbial processes, provided there are suitable oxidising species that the microbes can use to metabolise the hydrogen, but again, this is not considered likely to have any detrimental effect on repository safety.

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-Can is also indicated in the table and further described in Section 5.10.7.

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[6] If as a result sulphate were reduced to sulphide near the bentonite buffer surrounding a canister, then the sulphide might diffuse to the canister and cause corrosion of its copper surface.

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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	**Time period**	**Handling of influence**	**Influence present?**	**Time period**	**Handling of influence**
Temperature in bedrock	Yes. The solubility of gases is temperature dependent. The reaction/formation of gases would also be temperature dependent.	Excavation/operation,	Process neglected; no generation of repository gas expected.	Yes. But the effect of heats of solution/reaction is considered negligible.	Excavation/operation	Process neglected; little significance.
		Temperate	Gas generation and solubility at constant T in scoping calculations of gas transport in the geosphere, see Section 3.2.		Temperate	Influence neglected.
		Permafrost	Process not handled.		Permafrost	Process not handled.
		Glaciation	Influence neglected, little significance compared with other influences.		Glaciation	Influence neglected.
Groundwater flow	Yes. Flowing groundwater carries dissolved gasses.	Excavation/operation	Process neglected.	Yes. Trapped gas, the migration of gas bubbles, and instabilities in gas flow could affect groundwater flow.	Excavation/operation	Process neglected; little significance.
		Temperate	Considered in scoping calculations that bound the rate of generation of repository gas.		Temperate	Considered in scoping calculations of gas transport in the geosphere, see Section 3.2
		Permafrost	Process not handled.		Permafrost	Process not handled.
		Glaciation	Evaluation of the influence on inflow of oxygen with glacial melt waters.		Glaciation	Neglected, of little significance for groundwater flow.
Groundwater pressure	Yes. The solubility of gases is pressure dependent.	Excavation/operation	Process neglected; little significance.	Yes. The production of gases from wastes could raise groundwater pressure locally.	Excavation/operation	Process neglected; little significance.
		Temperate	Influence neglected, little significance.		Temperate	Neglected; based on results of scoping calculations.
		Permafrost	Process not handled.		Permafrost	Process not handled.
		Glaciation	Influence neglected; little significance.		Glaciation	Process neglected; little significance.
Gas 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 gas would increase the flow of the gas phase.	Excavation/operation	Process neglected; little significance.
		Temperate	Influence neglected; main gas is hydrogen released from the repository.		Temperate	Considered in scoping calculations of the capability of the geosphere to transport gas.
		Permafrost	Process not handled.		Permafrost	Process not handled.
		Glaciation	Influence neglected; little significance.		Glaciation	Gas flow neglected, see Section 3.2.
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 elevated gas pressure could disrupt the buffer or backfill.	–	–
Fracture geometry	Yes. Fracture geometry/connectivity controls gas migration.	All	See Section 3.2.	Yes. But only if the gas pressure rises enough to dilate/induce fractures.	All	See Section 3.2.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Rock stresses	No. But there could be an indirect effect through the effect of rock stresses on fracture properties/geometry.	–	–	Yes. In principle an elevated gas pressure could affect rock stresses, but not expected to be significant in fractured rock.	All	See Section 3.2.
Matrix minerals	No. But, indirectly weathering reactions will decrease the amount of dissolved O_2 and CO_2. This process is however slow.	–	–	No. But indirectly the dissolution of O_2 and CO_2 will induce reactions with minerals in the rock matrix. This process is however slow.	–	–
Fracture minerals	No. But indirectly some reactions will decrease the amount of dissolved O_2 and CO_2.	–	–	No. But indirectly the dissolution of CH_4, O_2 or CO_2 will induce microbial processes or reactions with minerals in the fracture surface.		
Groundwater composition	Yes. Gas solubility depends on groundwater salinity.	Excavation/operation	Process neglected; little significance.	Yes. Gaseous components are an integral part of groundwater composition.	Excavation/operation	Process neglected; little significance.
		Temperate	Constant salinity assumed in estimates of gas transport capacity in the geosphere.		Temperate	Scoping calculations of the amount of gas that could dissolve in the groundwater.
		Permafrost	Process not handled.		Permafrost	Process not handled.
		Glaciation	Considered in evaluation of oxygen consumption in glacial melt water.		Glaciation	Evaluation of oxygen consumption in glacial melt water.
Gas composition	Yes. Dissolved gas 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 gases produced in the groundwater.	Excavation/operation	Process neglected; little significance
		Temperate	Neglected; main gas is hydrogen released from the repository.		Temperate	Neglected; main gas is hydrogen released from the repository.
		Permafrost	Process not handled.		Permafrost	Process not handled.
		Glaciation	Neglected; little significance.		Glaciation	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 ground-water and react with concrete.	–	–
		Temperate	Neglected; little significance.			
		Permafrost	Neglected; little significance.			
		Glaciation	Neglected; little significance.			
Saturation	Yes. A gas phase would influence the dissolution of the gaseous components in a water phase.	Excavation/operation	Process neglected; little significance.	Yes. Gas generation might lead to a free gas phase, creating an unsaturated zone in the rock. However, this might be very localised.	All	See Section 3.2.
		Temperate	Solubility of gas considered in estimates of gas transport capacity in the geosphere.			
		Permafrost	Process not handled.			
		Glaciation	Neglected; little significance.			

5.10.3 Boundary conditions

The state of gases (dissolved or free gas phase) in the geosphere and the significance of their reactions depends on their concentrations. For natural gases, these depend on exchange with atmospheric gases near the surface, the fluxes of gases from deep 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.

Climate change, natural and anthropomorphic, 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 5.10.5).

Some processes will release gases and solutes from 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 2006fg/.

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). Where the surface is isolated from deep ground waters by permafrost, the infiltration of meteoric waters will be substantially reduced; this includes reduction in the transport of dissolved atmospheric gases to depth.

Permafrost conditions will lead to complex changes in the deep groundwater flow regime. 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-Can Climate report /SKB 2006e/.

The possible formation and decomposition of methane hydrates is discussed in Section 5.11.

5.10.4 Model studies/experimental studies

The solution 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 behave in these respects 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 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 time scales that need to be considered in a repository performance assessment. The gas generating potential of the cast iron in the waste containers and the predicted slow corrosion of this iron (should water contact the iron as a result of canister failure) mean also that gas could be produced from the wastes for a very long period.

The time scales for the transfer of gases, mainly H_2 from iron corrosion, from the repository tunnels and deposition holes into the geosphere are described in separate process description reports /SKB 2006fg/. The time scales relating to gas migration in the geosphere are discussed in Section 3.2.5.

5.10.6 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. 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.

5.10.7 Handling in the safety assessment SR-Can

The formation of hydrogen gas from a corroding cast iron insert in a defective canister is dealt with as part of the SR-Can safety assessment (see further report on Buffer/backfill processes /SKB 2006g/). 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.

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. Concentrations of dissolved natural gases are expected to remain substantially the same as those that exist now. Even during permafrost, natural gases that are continuosly 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. However, the formation of methane hydrates may not be completely excluded based on the site data available at present. In SR-Can, 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 and fracture filling minerals, as well as microbially mediated processes, see Sections 5.6 and 5.7.

5.10.8 Uncertainties

Uncertainties in mechanistic understanding

Understanding of the partitioning of gas between dissolved and free gas phases is good.

There is less certainty in the characterisation of the processes leading to the formation and distribution of natural gases. 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.

The main process, iron corrosion, that leads to gas generation in wastes, is satisfactorily well characterised. Gas generation from corrosion in waste packages will only occur if a canister defect allows water ingress into a canister. Uncertainties in the rate of water ingress leads 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 waste containers is a near-field process, it provides a source term for gas in the geosphere.

Model simplification uncertainties in SR-Can

Modelling the effects of gases in the geosphere is likely only to be considered in a simple way. As far as the processes considered in this overall section are concerned, formation, dissolution, and reaction of gases in the geosphere, little modelling is anticipated. The formation and reaction of natural gases will not be modelled, except for the modelling of the effect of the enhanced infiltration of oxygenated glacial melt waters during glacial periods. The partitioning of gases between dissolved and free gas phases will be 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.

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-Can

The coefficients that are needed to describe the partitioning of gas between dissolved and free gas phases are well known when the aqueous phase starts as 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 will require 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 Sections 5.5 and 5.6. Data uncertainties on the evaluation of microbially mediated processes are discussed in Section 5.7.

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
- 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 5-4 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.

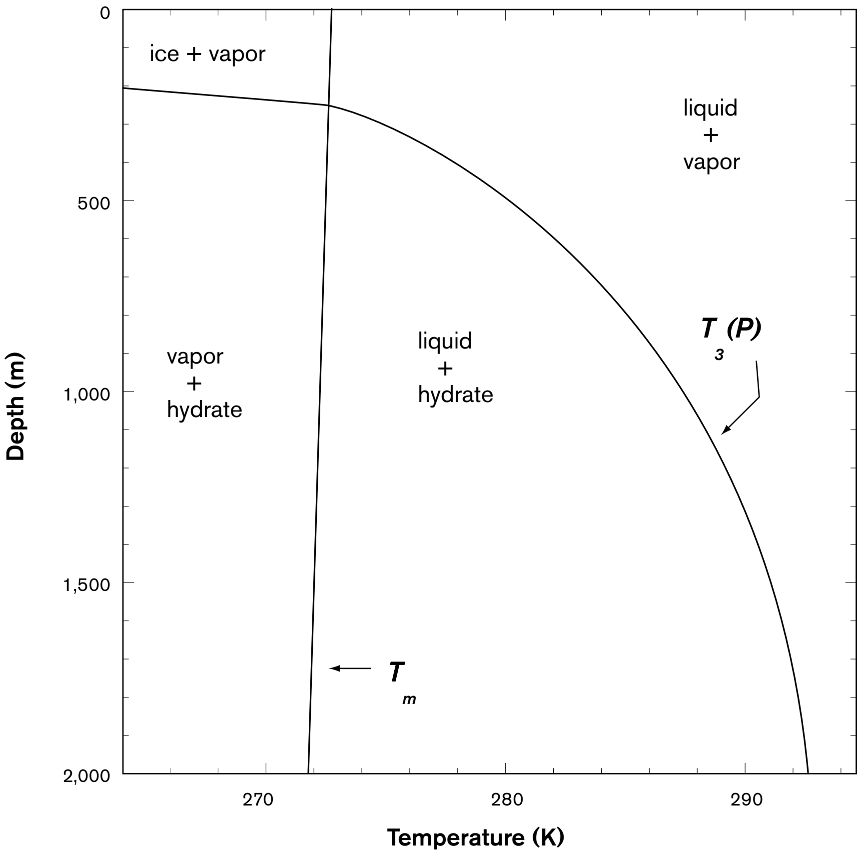

Figure 5-4. *Phase diagram for a methane-water mixture as a function of depth and temperature. Temperature $T_3(P)$ bounds the region where hydrate is stable and T_m is the melting temperature of pure water; after /Buffet 2000/.*

The role of temperature, when methane hydrate coexists with liquid solution, was underlined by /Zatsepina and Buffett 1997/, see Figure 5-5. 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 5-4). 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 5-6 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 c 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 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.

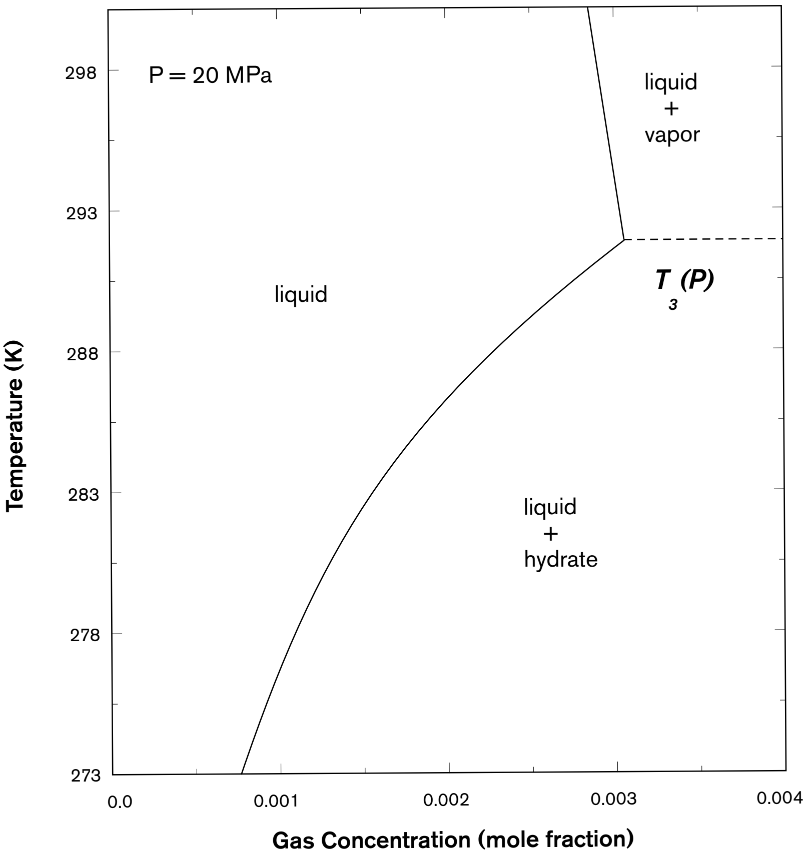

Figure 5-5. *Phase diagram for a methane-water mixture as a function of temperature and gas concentration. The solid line represents the solubility of gas in equilibrium with either vapour or hydrate; after /Buffett 2000/.*

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 5-4) 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 studied ice cores from the 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 of around 500 m /Ruskeeniemi et al. 2002, 2004/, although it is not certain whether this is a relict from the last Pleistocene glaciation or whether it is the cumulative result of several glaciations dating back hundreds of thousands of years.

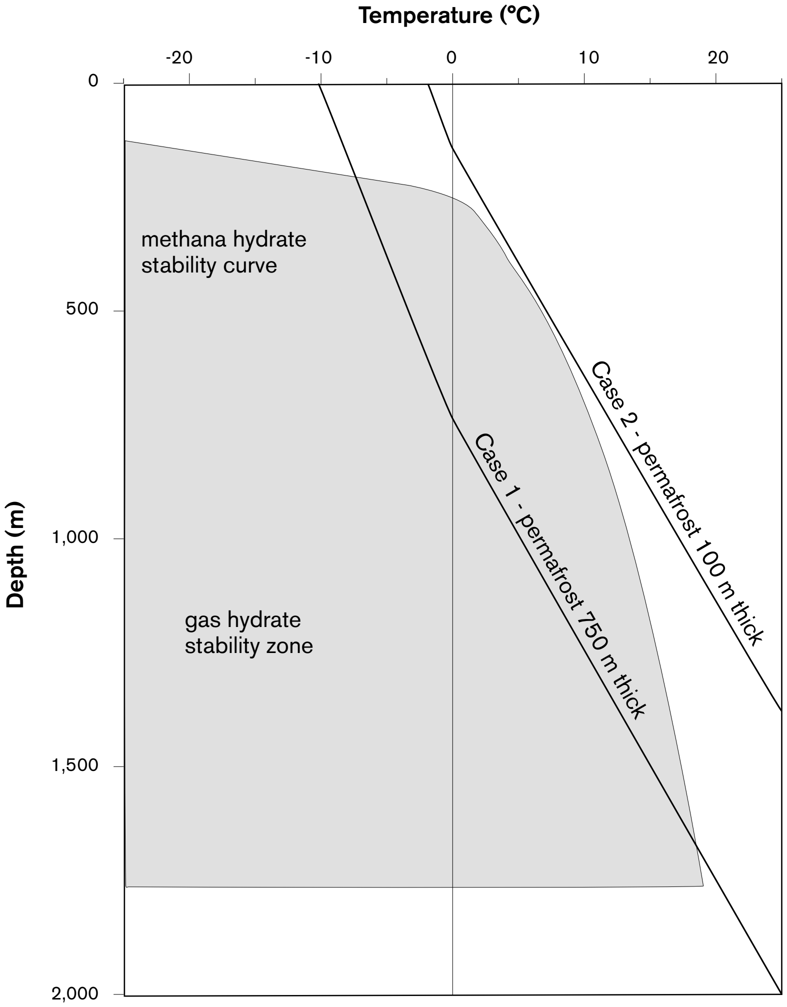

Figure 5-6. *Theoretical subsurface temperature profiles (geothermal gradient = 20°C/km) typical of the Canadian bedrock permafrost region superimposed on the methane hydrate stability curve (cf. Figure 5-4); after /Smith 2001/.*

However, 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 permafrost, SR-Can Climate report /SKB 2006e/. 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 into hydrates. In nature, methane hydrate has been observed in marine sediments and underneath permafrost (see below).

Repository implications

The main potential problem of large quantities of methane hydrate at or close to repository levels is the energy released during its dissociation when temperature increases and pressure decreases. At a repository location, there will be two sources of temperature increase: a) heat from the spent fuel packages, and b) heat from climate changes and the 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 widespread 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. If large quantities of methane hydrates are formed around or above the repository, their melting could potentially release large amounts of gaseous methane during a short time. It is not impossible that this would affect the hydraulic properties of the rock mass by inducing cracks or reactivating existing fractures.

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. 1991ab/, see also Figure 5-3.

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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes.	Permafrost Glaciation	Process not evaluated	Yes. By latent heat of melting/freezing.	Permafrost Glaciation	Process not evaluated.
Groundwater flow	No. But indirectly by advection of methane.	–	–	No. But indirectly by changing fracture geometries.	–	–
Groundwater pressure	Yes.	Permafrost Glaciation	Process not evaluated	Yes. By expansion of the ice.	Permafrost Glaciation	Process not evaluated.
Gas 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.	Permafrost Glaciation	Process not evaluated	Yes. By affecting porosity, and potentially methane hydrate may open up or expand fractures.	Permafrost Glaciation	Process not evaluated.
Rock stresses	No. But indirectly by affecting porosity.	–	–	Yes. By the expansion caused by the larger volume of methane ice, and possibly by large volumes of gas released on fast dissociation events.	Permafrost Glaciation	Process not evaluated.

Matrix minerals	No. But, indirectly through thermal properties of rock matrix.	–	–	No.	–	–
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.	Permafrost Glaciation	Process not evaluated.	Yes. The formation of methane hydrates would deplete surrounding groundwater from methane; and salt exclusion may occur.	Permafrost Glaciation	Process not evaluated.
Gas composition	Yes.	Permafrost Glaciation	Process not evaluated.	Yes. Removal of methane.	Permafrost Glaciation	Process not evaluated.
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.	Permafrost Glaciation	Process not evaluated.	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.	Permafrost Glaciation	Process not evaluated.

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/. That study focussed on the presence of a naturally occurring secondary ice phase to establish whether it is a dissociated unreacted ice phase, a dissociated ice product, or frozen pore water. Understanding the alteration evolution of naturally occurring hydrates during their transit to the surface 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.

5.11.5 Time perspective

Methane hydrates may only form under periods of permafrost or glaciation.

5.11.6 Natural analogues/observations in nature

Of the many observations documented, the Mallik site in the MacKenzie Delta, Northwest Territories, Canada, has been the focus of a major research programme, with the first research borehole drilled in 1998 by an international consortium /Dallimore and Collett 1995, 1999/. This was 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 physico-chemical understanding to the formation, stability and ultimate dissociation of these hydrate phases under similar permafrost conditions as expected during future climate change in Fennoscandia.

5.11.7 Handling in the safety assessment Sr-Can

Excavation/operation and Temperate periods

Methane hydrate formation cannot take place during these periods at a repository site.

Permafrost and Glaciation periods

Methane hydrate formation cannot be excluded during these periods at a repository site.

If freezing is deemed to be possible at repository depth, the effects of ice formation, and of methane ice formation, have to be evaluated.

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. Within SR-Can this possibility is not explored. More site data on methane concentrations and isotopic compositions are needed before this factor can be evaluated.

5.11.8 Uncertainties

Uncertainties in mechanistic understanding

Methane ice formation is a physically well understood process.

Model simplification uncertainties in SR-Can

Not relevant.

Input data and data uncertainties in SR-Can

Not relevant.

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 borderline between fresh and saline water at the depth to which the perennially frozen front has reached. Depending on the geometry of the groundwater-containing fracture system, pockets of saline, un-frozen 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 brine character (> 100 g/L TDS) and rich in sulphate. 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 (sulphate reducing bacteria). 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 saline groundwaters present in coastal areas of the Baltic Sea are the result of the freezing of seawater which may occur 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.

There is, therefore, evidence to assume that freeze-out processes most probably have influenced the Baltic region, but the extent is 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 can only be estimated through model calculation. In northern Canada, permafrost presently exists to around 500 m depth /Ruskeeniemi et al. 2002, 2004/, although it is not certain whether this is a relict from the last Pleistocene glaciation or whether it is the cumulative result of several glaciations dating back to hundreds of thousands of years, as is the case for the permafrost occurrences of N.E. Siberia which extend to 1,000 m depth and more. 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, SR-Can Climate report /SKB 2006e/.

One of the main geochemical indicators to trace the presence of permafrost freeze-out brines would be the preservation of sulphate-rich groundwaters resulting from the dissolution of mirabilite. Other possibilities include strong fractionation of $\delta^{18}O$ and ^{2}H producing lighter fractions than the original groundwaters /Ruskeeniemi et al. 2004/, the fractionation of boron isotopes producing high $\delta^{11}B$ signatures /Casanova et al. 2004/ and the formation of heavy $\delta^{13}C$ calcites /Clark and Lauriol 1992/. Unfortunately, because of flushing out and mixing of the groundwaters close to the Baltic Shield coastline following glacier decay and isostatic recovery, many of the freeze-out brines have either been removed or diluted or may have migrated to depth and mixed with existing brines. It is possible that some of the light $\delta^{18}O$ values measured at depths of 1,000 m are due to freeze-out brines and not due to a component of glacial melt water as normally proposed.

The best possibility to specifically detect the effects of permafrost activity is a mineralogical signature (e.g. associated with calcite) or finding by chance a preserved pocket/lens of brine in low permeable parts of the bedrock.

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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	Yes. The amount and composition of the saline water is temperature-dependent.	Permafrost Glaciation	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.	Permafrost Glaciation	Included in a generic model of groundwater flow under permafrost, see Section 3.1.
Groundwater pressure	Yes. Pressure affects the freezing temperature of water, and thus the exclusion of salts.	Permafrost Glaciation	Simplified and pessimistic assumption regarding the quantity of out-frozen salt (see Section 5.12.8).	No.	–	–
Gas 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.	Permafrost Glaciation	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.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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.	Permafrost Glaciation	Generic model of groundwater flow under permafrost assumes present day depth profile for salinity.	Yes.	Permafrost Glaciation	Groundwater salinities evaluated through a generic model of density-driven flow under permafrost.
Gas composition	No.			No.		
Structural and stray materials	No.	–	–	Yes. Potentially detrimental – chemical brine-induced degradation of cement and metal corrosion.	Permafrost Glaciation	Degradation of grout not evaluated for permafrost conditions in SR-Can, see Section 5.8.
Saturation	Yes.	Permafrost Glaciation	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 waters 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

As indicated above, experimental studies have been successful in producing brines by salt exclusion resulting from seawater freezing and evaporation, e.g. /Nelson and Thompson 1954, Thompson and Nelson 1956, Herut et al. 1990/. The main difference between freezing and evaporation of seawater is that the excluded sulphate ion forms mirabilite during freeze-out rather than forming gypsum (or anhydride) from evaporation. Recent work /Ruskeeniemi et al. 2004/ describes freezing experiments using waters other than seawater; a Na-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 showed an increasing trend towards greater concentrations and $\delta^{18}O$ and $\delta^{2}H$ became increasingly lighter. 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 Time perspective

Salt exclusion due to freezing may only occur under periods of permafrost or glaciation.

5.12.6 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/ and in the various site characterisation investigations being carried out in Sweden and Finland.

5.12.7 Handling in the safety assessment SR-Can

Excavation/operation and Temperate periods

Salt exclusion by freezing will not take place during these periods.

Permafrost and Glaciation periods

Generic calculations showing the evolution of saline waters under permafrost are used to evaluate the possible impact at repository level. 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.

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-Can

Modelling of the evolution of saline waters under permafrost, illustrating their downward movement due to density effects, is performed independently of the modelling of the advance of permafrost conditions. Thus, permafrost formation and salt exclusion is pessimistically assumed to take place instantaneously and homogeneously to a given depth, for example to 300 m, for the whole modelled site and all salt in the groundwater from the surface to the stipulated permafrost depth will be initially assumed to be present in a thin horizontal layer below the permafrost. Furthermore, in the illustrative calculations only one site will be used as an example, regional flow will be simplified and typical hydraulic parameters will be used. In a first stage, the effect of matrix diffusion is also neglected. The aim of the modelling exercise is to illustrate the process (density-driven groundwater flow) that prevents large accumulations of salt under a permafrost layer.

Salt exclusion might induce the precipitation of some minerals in fractures, e.g. mirabilite ($Na_2SO_4{\cdot}10H_2O$). This might affect fracture conductivity and groundwater flow. However, changes in hydraulic properties of fractures are not modelled in SR-Can.

Input data and data uncertainties in SR-Can

As the proposed modelling is intended to be used for illustrative purposes, a full exploration of the data uncertainties will not be carried out. The largest uncertainties are perhaps the salinity depth distribution of the original groundwater, and the extent, depth and propagation speed of the permafrost, as well as its local variations.

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. The canister wall is, however, sufficiently thick for the external effect of γ-radiolysis to be negligible.

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 the 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 2004f/. For the former, the grout should have an acceptably low hydraulic conductivity (e.g. $< 10^{-12}$ ms^{-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. 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 in the current context.

Although alpha radiation is the least penetrating of the three common types of radiation, it may become an important issue resulting from extensive sorption of radionuclides on existing fracture minerals and/or precipitation of secondary minerals of uranium in fractures. Over time, alpha radiation might locally degrade the rock fracture fillings and/or adjacent grouting material.

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-Can 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 flow	No.	–	–	Yes. Radiolysis may generate gas.	All	Process neglected; too low radiation fluxes.
Repository geometry	Yes. Will affect the spatial disposition of the radial flux 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.			No.		
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 /YMP 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 2.11×10^{13} n/cm^2 which is significantly less than required to cause any structural damage. According to /Elleuch et al. 1970/, no degradation of the mechanical properties of cement have been observed for fast neutron fluence as high as 8.2×10^{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 1.96×10^{8} MeV/cm^2-s /CRWMS M and 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 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.

5.13.5 Time perspective

This is determined by the decay properties of the spent fuel, see the SR-Can process report for fuel and canister /SKB 2006f/. The γ- and neutron-radiation fluxes leaving the canister are only significant for approximately the first 1,000 years.

5.13.6 Natural analogues/observations in nature

No observations of radiation damage on rock or cementitious materials have been reported from either observations in nature or studies of natural analogues.

5.13.7 Handling in the safety assessment SR-Can

Excavation/operation and Temperate periods

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.

Permafrost and Glaciation

Lower radiation fluxes are expected during these periods. Therefore, the process is neglected also during these periods.

5.13.8 Uncertainties

There are no uncertainties of relevance to the safety assessment.

5.14 Earth currents

5.14.1 Overview/general description

Earth (or telluric) currents are natural electric currents that flow on and beneath the surface of Earth (including the oceans) parallel to its surface. They arise as charges from different sources trying to reach equilibrium. Sources include low-frequency electromagnetic waves from space and charged masses in the ionosphere and atmosphere. Some of these phenomena are used by geophysicists to map subsurface structures, for example Magneto-Tellurics, which uses measurements of the two horizontal components of both the geomagnetic and geoelectric fields, and Geomagnetic-Depth sounding, which uses measurements of all three components of the geomagnetic field. With respect to geochemical processes, two main phenomena may be relevant: electrophoresis and electroosmosis. Electrophoresis is the separation of charged molecules or colloids using their different rates of migration in an electric field, and electroosmosis is the flow of an aqueous solution through a capillary or a porous medium under the influence of an electrical field, as opposed to that under a hydraulic pressure gradient. These two processes are also referred to as electrokinetic phenomena.

In the natural environment, the major influence of earth currents on geochemical processes appears to be confined to the surface soil layers and it is a very slow process. Reference to deeper bedrock environments has so far not been found.

Most of the published literature refers to in situ field or laboratory studies in which, for example, an enhanced electric field is used to speed up the migration of ionic species (e.g. /Chen et al. 1999/). This enhancement approach has been applied widely to the remediation of contaminants from fine-grained sediments. Other applications include laboratory electroosmosis or electromigration studies on Boom Clay to determine the apparent molecular diffusion coefficients of radionuclides /Maes et al. 1999/. They concluded that the results were in excellent agreement with classical migration experiments.

It is also known that earth currents may affect the corrosion of metallic objects such as rails. Corrosion has been observed in down-hole sampling equipment in a borehole at Forsmark, and the effect has been attributed to the influence of electric power cables. However, the electric potential fields that are required in order to achieve noticeable electrokinetic effects are much larger than those needed to induce metallic corrosion. Therefore, it appears that natural earth or telluric currents, whilst present, are relatively unimportant phenomena in the context of repository geochemistry. The possible effects on canister corrosion are discussed in the SR-Can process report for fuel and canister /SKB 2006f/.

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-Can is also indicated in the table and further described in Section 5.14.7.

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”.

Table 5-15. Direct dependencies between the process "Earth currents" and the defined geosphere variables and a short note on the handling in SR-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 should be negligible.	–	–
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 should be negligible.	–	–
Gas flow	No.	–	–	No. But indirectly through the groundwater flow created by electro-osmosis. The effect should be negligible.	–	–
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.		
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.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 ground-water flow or solute transport.	No.	–	–

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-Can

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. Therefore these processes are not considered in SR-Can.

5.14.8 Uncertainties

Uncertainties in mechanistic understanding

Electrophoresis and electroosmosis are well understood processes.

Model simplification uncertainties in SR-Can

Not relevant.

Input data and data uncertainties in SR-Can

Not relevant.

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-Can process report for fuel and canister /SKB 2006f/).

In this section, the integrated aspects of these processes and their handling in the safety assessment SR-Can are discussed. The main transport processes of radionuclides and the modelling of those processes have been the focus of a recently finalised EU-project /RETROCK 2004, 2005/ involving both implementers, including SKB, and a regulator. The approach adopted in SR-Can and described below is heavily based on the RETROCK conclusions. The general description in the following paragraphs is also taken, in shortened form, 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 transport resistance or hydrodynamic control of retention. 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. In the more 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 $\int dl/(v(l)b(l))$ 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.

Matrix diffusion is caused by random movement, which, in the presence of concentration gradients, causes a net movement of solute. It is not exactly known how deep in the rock matrix the pores are connected, but some studies suggest this can occur to depths of at least tens of centimetres. 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 inhibit matrix diffusion. Another potentially inhibiting 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. 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 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 off 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-Can is also indicated in the table and further described in Section 6.1.7.

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-Can, see below.

The outer boundary is the geosphere-biosphere interface zone, or alternatively, the lateral and/or bottom boundary of the simulation domain for groundwater flow.

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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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.			
		Permafrost	RN-transport not considered for permafrost in SR-Can.			
		Glaciation	See Temperate above.			
Groundwater flow	Yes. Groundwater flow governs transport.	Excavation operation	Process not relevant.	No.	–	–
		Temperate	Flow paths, Darcy velocity, transport resistance, advective travel time from site-specific groundwater flow modelling, see Section 3.1			
		Permafrost	Process not considered in SR-Can.			
		Glaciation	Flow paths, Darcy velocity, transport resistance, advective travel time from site-specific groundwater flow modelling (only Laxemar in SR-Can), see Section 3.1.			
Groundwater pressure	No. But indirectly since pressure affects flow.	–	–	No.	–	–
Gas flow	No. But indirectly, since gas flow affects groundwater flow.	–	–	No. Does not affect gas flow (per definition).	–	–
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.			
		Permafrost	Process not considered in SR-Can.			
		Glaciation	Flow paths, Darcy velocity, transport resistance, advective travel time from simplified site-specific groundwater flow modelling (only Laxemar in SR-Can), see Section 3.1			

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Fracture geometry	Yes. Fracture network geometry governs flow and hence non-reactive transport characteristics.	Excavation operation	Process not relevant.	No. But indirectly since deposition of transported material may change fracture geometry. Also, reactions may change geometry by surface alteration (precipitation etc).		
		Temperate	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.			
		Permafrost	Process not considered in SR-Can.			
		Glaciation	Flow paths, Darcy velocity, transport resistance, advective travel time from simplified site-specific groundwater flow modelling (only Laxemar in SR-Can), see Section 3.1			
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 and also the extent of diffusion.	Excavation operation	Process not relevant.	No. If reactions occur, mineral changes could occur, but considered second order effect.	–	–
		Temperate	Site-specific rock mineralogy considered in the selection of sorption data, see Section 5.4.			
		Permafrost	Process not considered in SR-Can.			
		Glaciation	See Temperate above.			
Fracture minerals	Yes. Fracture minerals affect fracture surface sorption and also access to matrix through diffusion.	Excavation operation	Process not relevant.	No. If reactions occur, mineral changes could occur, but considered second order effect.	–	–
		Temperate	Site-specific fracture mineralogy considered in the selection of sorption data, see Section 5.4. However, surface sorption not invoked in SR-Can.			
		Permafrost	Process not considered in SR-Can.			
		Glaciation	See Temperate above.			

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Groundwater composition	Yes. Composition affects radio-elemental speciation of radionuclides, and hence their transport characteristics.	Excavation operation	Process not relevant	Yes. Transport of dissolved species affects the water composition, but trace element transport is not of importance to understand major chemistry.	Excavation operation	Process not relevant.
		Temperate	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.		Temperate	Radionuclide concentration and release to the biosphere are calculated.
		Permafrost	Process not considered in SR-Can.		Permafrost	Process not considered in SR-Can.
		Glaciation	See Temperate above.		Glaciation	See Temperate above.
Gas composition	No. But indirectly through dissolution in groundwater some gases (e.g. O2, CO2 and H2) affect radio-element 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	Process not relevant.	No.	–	–.
		Temperate	Sorption on structural and stray materials in the geosphere neglected.			
		Permafrost	Process not considered in SR-Can.			
		Glaciation	See Temperate above.			
Saturation	No. But indirectly, since saturation affects groundwater flow.	–	–	No.	–	–

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 of relevance for performance assessment do not exist. However, for shorter scales, the TRUE-1 /Winberg et al. 2000/ and TRUE Block scale /Poteri et al. 2002, Winberg et al. 2002, Neretnieks and Moreno 2003/ experiments have shed light on the predictive capability using models based on the same processes as described above.

Model studies for spatial and temporal scales of relevance for safety assessment have been performed in earlier performance assessment studies (e.g. SR 97 and SR-Can Interim), but most notably in the ongoing Task 6 of the Äspö Task Force on modelling of groundwater flow and transport of solutes /Hodgkinson and Black 2005/. 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. The type of processes that typically dominate tracer experiments (e.g. sorption on fracture surfaces and diffusion into stagnant zones of small volume) are not of interest on the longer time scales.

6.1.5 Time perspective

All timescales after canister failure are relevant for transport of radionuclides in the water phase.

6.1.6 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/.

6.1.7 Handling in the safety assessment SR-Can

Excavation/operation period

The process is of no relevance for this period, since the engineered barriers are considered to be intact.

Temperate period

The most detailed analysis of radionuclide transport is performed for the Temperate period. The modelling of this period, which is exemplified in the SR-Can Interim report /SKB 2004e/, is based on the code FARF31/Norman and Kjellbert 1990/. 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 are the Darcy velocity at the canister deposition holes, and the 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 stream tubes) 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. In the matrix, the radionuclides are subject to sorption described with the linear equilibrium K_d concept. The main simplifications made are that only steady-state flow-fields can be handled, and that decay-chains can only be handled for the case of homogeneous flow-related transport (i.e. flow-wetted surface) and rock matrix parameters. 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.

The validity of the assumption of steady-state flow in the transport calculations is assessed by transient particle tracking in the groundwater flow models. The retention processes cannot be fully incorporated in these analyses; only equilibrium sorption using a retardation coefficient can be used to mimic the slower solute transport rate relative to the water transport rate. Initial development work is on-going to formulate transport models which can handle both transient flow and arbitrary heterogeneity in rock matrix and flow-related transport parameters /Moreno et al. 2004, 2005, Neretnieks 2005ab, Painter et al. 2006/. However, this development should be seen as supporting modelling on the time scale of SR-Can.

Colloidal transport, which is not included in FARF31, can be handled using a finite volume version of FARF31 denoted FARF32 /Vahlund and Hermansson 2004/. In FARF32, 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.

Separate FARF31 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.

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-Can assessment /SKB 2006d/. Also the tunnel layout is needed for assigning starting positions for particles in the groundwater flow model.

Permafrost

The main objective of the permafrost simulations carried out within SR-Can is to assess the groundwater flow pattern during a period when the upper part of the geosphere may be frozen and thus restricted with respect to flow. No detailed calculations of radionuclide transport during permafrost conditions are undertaken, but bounding calculations in order to estimate radionuclide dose levels are carried out.

Glaciation

The simulation of groundwater flow during a glaciation cycle aims at establishing groundwater flow patterns during the glaciation build-up and retreat. A large super-regional domain needs to be considered for these simulations.

Radionuclide transport calculations during glacial conditions are carried out using the same approach as for the calculations during the temperate period. However, parameter choices will reflect the relevant conditions in terms of flow path and matrix interaction parameters.

Earthquakes

The potential impact of earthquakes is illustrated by simple calculations where no credit is taken for radionuclide retention in the geosphere, since shear displacement is expected to occur in the larger fractures, where the transport resistance is low.

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-Can

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 values of the Peclet number to be used are uncertain, but in SR-Can a range of values or a probabilistic approach is used. The effect of this uncertainty on the resulting transport characteristics is, however, small.

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-Can, channelling factors are applied to account for this uncertainty.

Concerning sorption, the uncertainties are more of a mechanistic nature than related to modelling. Specifically, 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. However, the process is of limited relevance for the overall safety of the repository, since high concentrations of colloidal material rarely occur naturally in the site-specific groundwaters of interest. Consequently, these uncertainties are not problematic in a safety assessment context.

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-Can

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-Can Data report /SKB 2006d/. The sorption and diffusion data, which are based on the site-descriptive models and a general assessment of existing data and associated uncertainties, are also presented in supporting documents /Crawford et al. 2006, Liu et al. 2006/ to the SR-Can Data report. 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-Can Data report /SKB 2006d/. The main uncertainties are related to the fact that in situ sorption data are not available, and different laboratory techniques are 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 ^{79}Se), and the Peclet number is varied as described above.

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. 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.

As described in Section 5.10.1, 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 one 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 /SKB 2004d, 2005b/, 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 6-2.

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. 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.

Table 6-2. Measured dissolved natural gas concentrations and estimated solubilities at the possible repository depth of 400m.

Gas	Measured concentration (mol m^3)	Approximate solubility at a depth of 400 m (mol m^3)
Nitrogen	< 5	31
Helium	< 1	15
Methane	< 0.006	72
Carbon dioxide	< 0.2	1,900
Hydrogen	< 0.01	33

6.2.2 Dependencies between process and geosphere variables

Table 6-3 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-Can 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 6-3. 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-Can.

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
Temperature in bedrock	No. But indirectly through gas flow and gas composition since temperature affects viscosity, density, and gas solubility.	–	–	No.	–	–
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 flow	Yes. Gas flow governs transport in gas phase.	Excavation operation Temperate Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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 Permafrost Glaciation	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 Permafrost Glaciation	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 species have been identified that could do this to a significant degree.	–	–

Variable	Variable influence on process			Process influence on variable		
	Influence present?	Time period	Handling of influence	Influence present?	Time period	Handling of influence
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 Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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.	–	–
Fracture minerals	Yes. Fracture minerals affect fracture surface sorption and also access to matrix through diffusion.	Excavation operation Temperate Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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 Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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 Permafrost Glaciation	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 Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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 Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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 Permafrost Glaciation	Process not relevant. Not considered since geosphere is short circuit 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 concentration 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 "sees". 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.

6.2.5 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.

6.2.6 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.

6.2.7 Handling in the safety assessment SR-Can

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 permafrost and glaciation periods

In the safety assessment, transport in the gas phase is treated pessimistically as a short circuit of the repository with 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.

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-Can

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 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.

Input data and data uncertainties in SR-Can

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 are likely, on the basis of past assessments, to 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.

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