Technical Report

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Geosphere process report for the safety assessment SR-PSU

Svensk Kärnbränslehantering AB

November 2014

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Preface

This report compiles information on processes in the geosphere that are relevant for the long-term safety of the SFR repository. The report forms part of the SR-PSU safety assessment, which supports SKB's licence application to extend SFR.

This report has been compiled and edited by Teresita Morales, SKB and Martin Löfgren, Niressa. The experts that have contributed are listed in Section 1.7.

Members of the SR-PSU internal review panel named SARG and colleagues at the division of Research and Safety assessment at SKB have reviewed the report.

Stockholm, November 2014

Fredrik Vahlund
Project leader SR-PSU

Summary

The final repository for short-lived radioactive waste (SFR) located in Forsmark, Sweden is currently being used for the final disposal of low- and intermediate-level operational waste from Swedish nuclear facilities. SKB plans to extend the repository to host waste from the decommissioning of the nuclear power plants. The SR-PSU assessment of the long-term safety (post-closure safety) of the whole repository is an important part of the application for a license to build the extension. This process report constitutes one of the main references supporting the **Main report**, which summarises the long-term safety for SFR. Processes that are expected to take place in the geosphere of SFR in the period up to 100,000 years post-closure are systematically documented in this process report, including an evaluation of the importance of each process within the SR-PSU and a suggestion of how the process should be handled in the SR-PSU activities. This report addresses processes related to the geosphere. The process report supports the description of the repository long-term reference evolution. This report consists of five main chapters describing the geosphere processes.

Sammanfattning

Slutförvaret för kortlivat radioaktivt avfall (SFR) i Forsmark, Sverige används för närvarande för slutlig deponering av låg- och medelaktivt driftavfall från svenska kärntekniska anläggningar. SKB planerar att bygga ut förvaret för att förvara avfall från rivning av kärnkraftverken. Analysen av långsiktig säkerhet SR-PSU (säkerhet efter förslutning) för hela förvaret är en viktig del av ansökan om att få bygga ut förvaret. Den här processrapporten utgör en av huvudreferenserna till huvudrapporten som summerar analysen av långsiktig säkerhet för SFR. Processer som förväntas ske i geosfären i SFR under 100 000 år efter förslutning dokumenteras systematiskt i denna processrapport, vilken inkluderar utvärdering av varje process betydelse och förslag om hur processen ska hanteras inom SR-PSU. Den här rapporten behandlar processer för geosfären. Processrapporten är en viktig del i underlaget för beskrivningen av förvarets referensutveckling. Rapporten är indelad i fem huvudkapitel som beskriver de relevanta processerna för geosfären.

Contents

1 Introduction

1.1 Background

The final repository for short-lived radioactive waste (SFR) located in Forsmark, Sweden is currently in operation for the final disposal of low- and intermediate-level operational waste from Swedish nuclear facilities. SKB plans to extend SFR to host waste from the decommissioning of the nuclear power plants and other nuclear facilities. Additional disposal capacity is needed also for operational waste from nuclear power units since their operation life-times have been extended compared with what was originally planned.

An analysis of the long-term post closure safety of the whole SFR is needed as a part of SKB's licence application to extend and continue to operate SFR. This has been assessed and documented in the **Main report** with supporting documents, see Section 1.2. An overall description of the methodology of the safety assessment is given in the **Main report** (Chapter 2).

The present report is one of the main references to the **Main report** and describes the thermal, hydraulic, mechanical and chemical processes in the geosphere that are relevant for the long-term safety of SFR.

The SFR repository includes waste vaults located 60 metres underground the Baltic Sea, together with buildings above ground that include a number of technical installations. The existing facility (SFR 1) comprises five waste vaults with a disposal capacity of approximately 63,000 m^3. The extension (SFR 3[1]) will be built at 120 metres depth and will have a disposal capacity of 108,000 m^3 in five new waste vaults plus one new vault for nine boiling water reactor pressure vessels, see Figure 1-1.

The extension is called SFR 3 since the name SFR 2 was already used in a previous plan to build vault adjacent to SFR 1 for the disposal of a reactor core component and internal parts. The current plan is to dispose of the reactor core components and reactor internal parts in a separate repository.

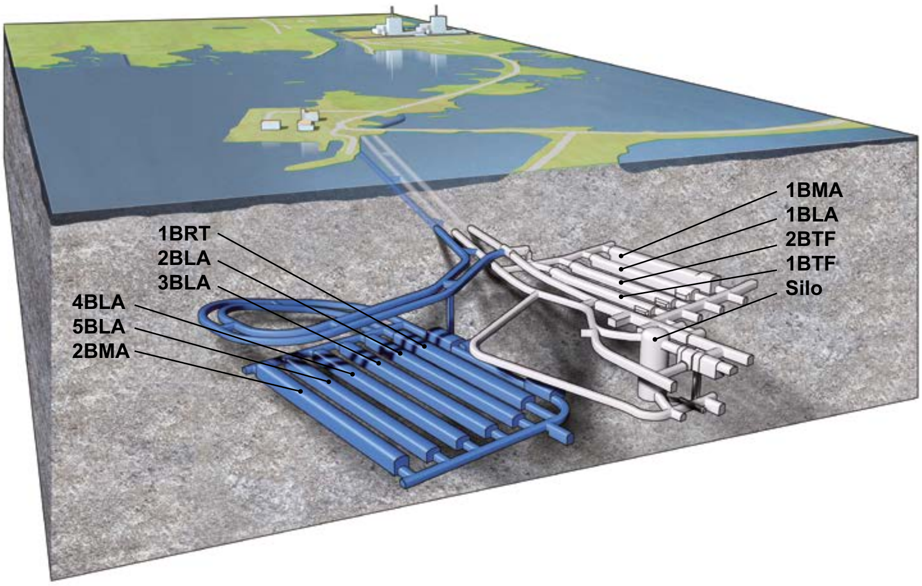

Figure 1-1. *Schematic illustration of SFR. The grey part is the existing repository (SFR 1) and the blue part is the planned extension (SFR 3). The waste vaults in the figure are the silo for intermediate-level waste, 1–2BMA vaults for intermediate-level waste, 1–2BTF vaults for concrete tanks, 1–5BLA vaults for low-level waste and the BRT vault for reactor pressure vessels.*

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[1] The extension is called SFR 3 since the name SFR 2 was used in a previous plan to build vaults adjacent to SFR 1 for disposal of reactor core components and internal parts. The current plan is to dispose of this waste in a separate repository.

1.2 Report hierarchy in the SR-PSU safety assessment

The documentation of the long-term post closure safety of the whole SFR is contained in the **Main report** with supporting documents. The **Main report** is part of SKB's licence application to extend and continue to operate SFR (**Main report**, Section 1.1). The present report is one of the main references providing a scientifically and justified plan for handling geosphere processes relevant for the long-term safety of SFR.

A schematic illustration of the safety assessment documents is shown in Figure 1-2.

There are also a large number of additional references. The additional references include documents compiled within SR-PSU, but also documents compiled outside of the project, either by SKB or equivalent organisations as well as in the scientific literature. Additional publications and other documents are referenced in the usual manner.

The applied methodology for the long-term safety comprises ten steps and is mainly described in Chapter 2 of the **Main report** of SR-PSU. However, several steps carried out in the safety assessment are described in more detail in th so called Main references that are of central importance since they support conclusions and analyses in the **Main report**. The full titles of these main referende reports and their abbreviations (in bold font) are given in Table 1-1, together with a short summary of the contents of the reports.

1.3 This report

The **Geosphere process report** is a product of step 4 – Description of processes, and identified as relevant for the long-term safety in Step 1 – Handling of FEP's (Features, Events and Processes), in the applied methodology for the long-term safety (**Main report**, Section 2.4).

The purpose of the **Geosphere process reports** is to document the scientific knowledge of the processes to a level required for an adequate treatment of processes in the safety assessment. The documentation is not exhaustive from a scientific point of view, which is not the purpose of the process report but to give a comprehensive background relevant for the actual and further handling of the process itself, within the assessment. A certain process needs to be sufficiently described and documented as proven well understood, so it can serve the necessary purposes to answer specific questions, and associated uncertainties, based on arguments founded on scientific understanding. Further, the treatment of each process in the safety assessment is described and the methodologies established and applied in the consequent handling in the safety analysis; i.e. the reference evolution (step 7), scenario analysis (step 9) and radionuclide transport calculations.

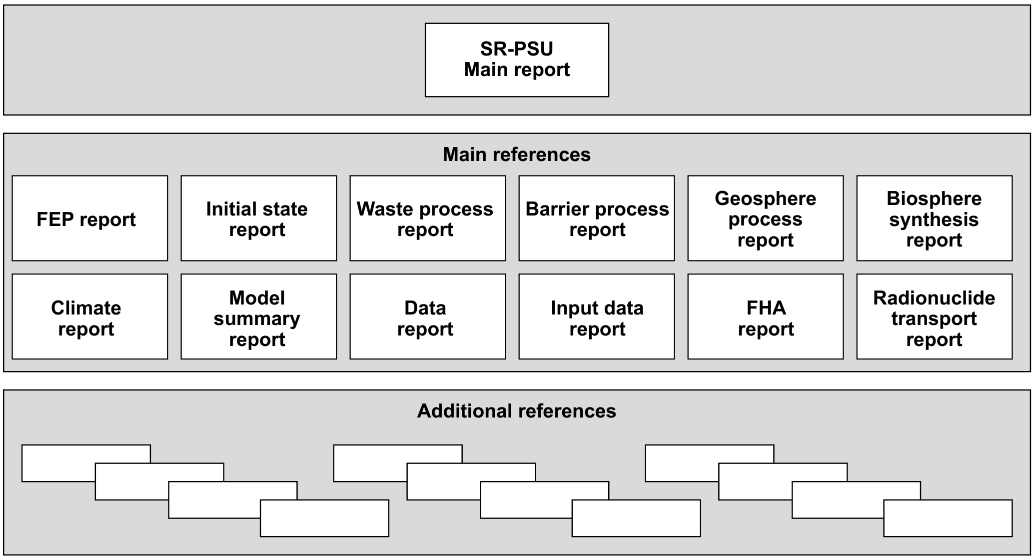

*Figure 1-2. The hierarchy of the **Main report**, Main references and additional references in the SR-PSU long-term safety assessment. The additional references either support the **Main report** or any of the Main references.*

Table 1-1. Main report and Main references in the SR-PSU long term safety assessment. All reports are available at www.skb.se

Abbreviation used when referenced in this report	Text in reference list	Comment on content
Main report	**Main report, 2014**. Safety analysis for SFR. Long-term safety. Main report for the safety assessment SR-PSU. SKB TR-14-01, Svensk Kärnbränslehantering AB.	This document is the main report of the SR-PSU long-term post-closure safety assessment for SFR. The report is part of SKB's licence application to extend and continue to operate SFR.
Barriers process report	**Engineered barriers process report**, **2014**. Engineered barrier process report for the safety assessment SR-PSU. SKB TR-14-04, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of the processes in the engineered barriers that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. Reasons are given in the process report as to why each process is handled a particular way in the safety assessment.
Biosphere synthesis report	**Biosphere synthesis report**, **2014**. Biosphere synthesis report for the safety assessment SR-PSU. SKB TR-14-06, Svensk Kärnbränslehantering AB.	Describes the handling of the biosphere in the safety assessment. The report summarises site description and landscape evolution, FEP handling, exposure pathway analysis, the radionuclide model for the biosphere, included parameters, biosphere calculation cases and simulation results.
Climate report	**Climate report**, **2014**. Climate and climate-related issues for the safety assessment SR-PSU. SKB TR-13-05, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of climate and climate-related processes that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. The report also describes the climate cases that are analysed in the safety assessment.
Data report	**Data report, 2014.** Data report for the safety assessment SR-PSU. SKB TR-14-10, Svensk Kärnbränslehantering AB.	Qualifies data and describes how data, including uncertainties, that are used in the safety assessment are quality assured.
FEP report	**FEP report, 2014.** FEP report for the safety assessment SR-PSU. SKB TR-14-07, Svensk Kärnbränslehantering AB.	Describes the establishment of a catalogue of features, events and processes (FEPs) that are of potential importance in assessing the long-term functioning of the repository.
FHA report	**FHA report**, **2014**. Handling of future human actions in the safety assessment SR-PSU. SKB TR-14-08, Svensk Kärnbränslehantering AB.	Describes radiological consequences of future human actions (FHA) that are analysed separately from the main scenario, which is based on the reference evolution and less probable evolutions.
Geosphere process report	**Geosphere process report**, **2014**. Geosphere process report for the safety assessment SR-PSU. SKB TR-14-05, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of the processes in the geosphere that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. Reasons are given in the process report as to why each process is handled a particular way in the safety assessment.
Initial state report	**Initial state report**, **2014**. Initial state report for the safety assessment SR-PSU. SKB TR-14-02, Svensk Kärnbränslehantering AB.	Describes the conditions (state) prevailing in SFR after closure. The initial state is based on verified and documented properties of the repository and an assessment of the evolution during the period up to closure.
Input data report	**Input data report**, **2014**. Input data report for the safety assessment SR-PSU. SKB TR-14-12, Svensk Kärnbränslehantering AB.	Describes the activities performed within the SR-PSU safety assessment and the input data used to perform these activities.
Model summary report	**Model summary report**, **2014**. Model summary report for the safety assessment SR-PSU. SKB TR-14-11, Svensk Kärnbränslehantering AB.	Describes the calculation codes used in the assessment.
Radionuclide transport report	**Radionuclide transport report**, **2014**. Radionuclide transport and dose calculations for the safety assessment SR-PSU. SKB TR-14-09, Svensk Kärnbränslehantering AB.	Describes the radionuclide transport calculations carried out for the purpose of demonstrating fulfilment of the criterion regarding radiological risk.
Waste process report	**Waste process report, 2014.** Waste form and packaging process report for the safety assessment SR-PSU. SKB TR-14-03, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of the processes in the waste and its packaging that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. Reasons are given in the process report as to why each process is handled in a particular way in the safety assessment.

1.3.1 Overall methodology of SR-PSU

The detailed assessment methodology, including the role of the process reports in the assessment, is described in the **Main report**. The following points summarise the overall assessment methodology, and clarify the intended work process of SR-PSU, and hence the role of process reports in general.

The repository system is broadly defined as the deposited operational and decommissioning waste, the engineered barriers surrounding the waste, the host rock and the biosphere at the surface. Future states and the evolution of the system will depend on:

- The initial state of the system (see Section 1.5).
- A number of related thermal, hydraulic, mechanical and chemical processes acting within the system over time.
- External conditions influencing and/or acting on the system.

A methodology involving ten steps has been applied for SR-PSU, illustrated as follow:

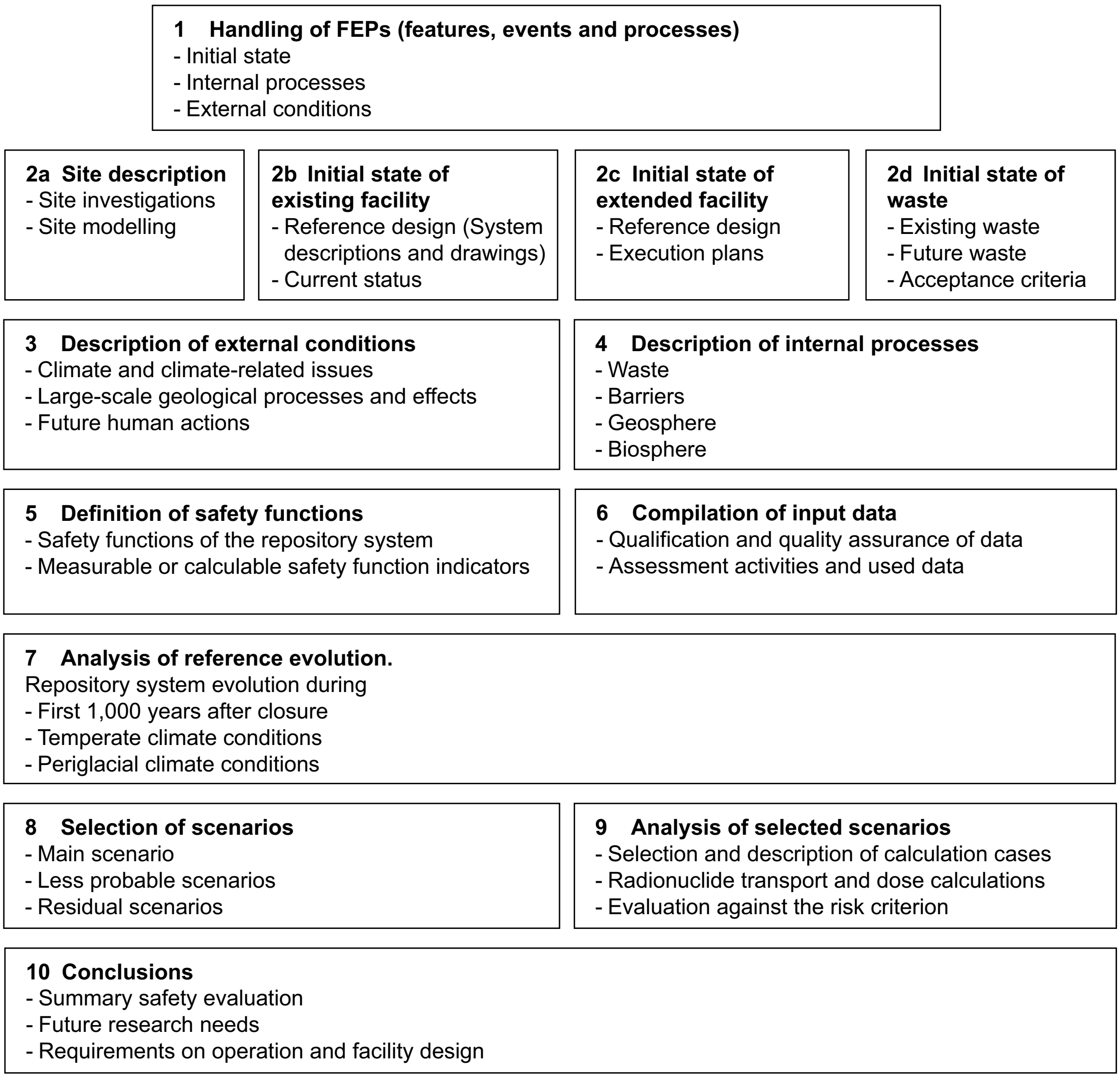

***Figure 1-3.** Overview of the ten steps in the methodology used for the long-term safety assessment SR-PSU.*

1.4 Identification of geosphere processes

This is the first time SKB has compiled a process report for the geosphere regarding the repository for low- and intermediate waste in SFR. The **Geosphere process report** was initiated straight after the completion of the SR-Site report and therefore profited from much of the work already performed. Large-scale geological processes are described in the SR-Site Geosphere process report (SKB 2010e). Since both repositories are planned to be located in Forsmark, these descriptions apply also for SFR.

For the SR-PSU safety assessment the FEP lists and databases have been revisited (**FEP report**). A complete list of processes described in the SR-PSU process reports can be found in the abovementioned **FEP report**.

1.4.1 FEPs mapped to the geosphere process system

For SR-PSU, a renewed FEP processing has been performed using all project FEPs in the international NEA FEP database version 2.1 (NEA 2006) resulting in lists of NEA FEPs mapping to present system related processes. These FEP lists have been checked in order to ensure that all relevant aspects of each process is addressed in the process descriptions and handled appropriately in the SR-PSU assessment. The handling of each FEP has been documented in tables created for this purposeand provided in the **FEP report**.

FEPs related to large-scale geological processes

The large-scale mechanical evolution of the shield includes tectonic uplift, seismicity due to plate tectonic relaxation resulting in earthquakes, are better described in the SR-Site Geosphere process report (SKB 2010e, Sections 4.1.2 and 4.1.3, respectively). These descriptions apply also for SFR.

1.4.2 Definition of the geosphere system and variables

The repository system is divided into three system components; the waste and the technical barriers (consisting parts of the "near-field"), the geosphere (the hard rock, consist partly the "far-field") and the biosphere (mainly the surface regardless type of the type of "sphere"). For each component of the repository system, a list of processes is established.

The boundaries of the geosphere system

In previous assessments, (SAR-08 and SAFE) the geosphere constituted one system component. A provisional definition of the geosphere system was given in the SAFE project and SAR-08 (SKB 2001b, SKB 2008b): "The geosphere matrix represents the rock and tunnel system. The upper extension of the system is from the rock walls in the Silo and repository vaults up to an arbitrary border between deeper rock and surface rock. The surface rock, mainly in terms of outcrops, is included in the biosphere matrix in order to facilitate the treatment of the geosphere/biosphere interface. The horizontal and depth extension of the system is an arbitrary distance into the rock surrounding the repository vaults."

Previous definition of the geosphere system within the safety assessment SR-Can (SKB 2006b): "Geosphere. This system component comprises the rock surrounding the repository and the investigation boreholes. It also includes grout injected into fractures in the rock during construction of the repository to prevent water inflow to tunnels and other repository cavities. In the upward direction, the geosphere is bounded by 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 boundaries in the other directions, see definitions above regarding the system boundary."

For a deep geological repository it is possible to separate the geosphere into deep and near surface geosphere. However, for a shallow geological repository such as SFR, this division is not relevant and the repository geosphere is considered to consist only of near-surface geosphere.

The boundaries between different system components of the repository system, i.e. between the waste and technical barriers, the geosphere and the biosphere, are defined in detail by the responsible experts and modellers for each subject area. However due to the different questions set for the different subject areas, these boundary conditions may differ between the various models performed within each subject area and hence, between system components. However the processes are structured, separately, within each system component.

The boundary between the bedrock and the loose overburden used in hydrogeological modelling of the groundwater flow may for example differ from the lower boundary used in surface hydrological modelling of the groundwater flow , where part of the bedrock is included.

Variables

The physical variables required to describe the properties and conditions of the geosphere processes are listed in Table 1-2. The variables are then used for addressing the interaction of each process. If the variable and process interaction has been judged to be potentially important for the geosphere; a method of handling them is suggested and summarised (see Chapter 7 and the **FEP report**).

Table 1-2. List of variables and definition of these variables.

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 geospere's fracture system.
Gas phase flow	Gas phase flow as function of time and space in the geosphere fracture system.
Repository geometry	Geometric description of caverns, silo, tunnels, ramps, boreholes etc i.e. of all excavated volumes.
Fracture and pore geometry	Geometric description of all cavities, from fracture zones to micro-pores in the rock matrix.
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 materials that occur. Also the amount and composition of these fracture-filling materials.
Groundwater composition	Chemical composition of the groundwater as a function of time and space, i.e. redox, pH, ionic strength, concentration of dissolved species, type and amount of colloid particles, amount and composition of dissolved gas, radionuclides, density, viscosity.
Gas composition	Chemical composition of gases in geosphere cavities including any radionuclides located in fractures in the rock and left there at repository closure.
Structural and stray materials	Chemical composition and quantities of grouts and other structural and stray materials injected.
Saturation	Degree of water saturation of the geosphere.

1.5 Geosphere initial state and evolution

1.5.1 External conditions and geosphere processes

External conditions affecting the geosphere and the rock surrounding the repository during its lifetime are climate variations and indirect effects of climate change (**Climate report**). Large-scale processes, such as earthquakes (due to plate tectonic, tectonic uplift and seismicity) may also influence the geosphere and the rock surrounding the repository during its lifetime and discussed elsewhere (see Section 1.4.1 and Section 4.1.2). Further, geosphere processes considered related to external conditions are weathering, erosion and sedimentation, acting and affecting the geosphere on time-scales of millions to hundreds of millions of years. However, these processes are not explicitly described in this report but implicitly considered i.e., denudation and relative shore-level displacement due to isostatic and eustatic sea-level variation (**Climate report**). Erosion and sedimentation, groundwater recharge and discharge, soil formation, primary production, and decomposition of organic matter are included in the description and modelling of landscape development (**Biosphere synthesis report**).

Geological setting

The episodes of tectonic uplift that formed the current Fennoscandian topography occurred mainly during the Tertiary (from 1.8 to 65 million years ago). The Scandinavian mountain chain and the southern Swedish highlands formed as a result of these episodes (see e.g. Lidmar-Bergström and Näslund 2002). Increased erosion and weathering due to tectonic uplift and repeated episodes of subglacial erosion during the Tertiary to the prehistoric, led to the formation of a smooth bedrock surface. As a result, the crystalline bedrock originating before the Cambrian was re-exposed. Although this smooth bedrock surface, called the sub-Cambrian peneplain, is somewhat fractured along major fracture zones in the Forsmark area, the tectonic conditions have remained stable in the area during the past 1.8 million years (Lidmar-Bergström and Näslund 2002, Olvmo 2010). During this period, isostatic changes, caused by glacial loading and unloading, have instead been crucial for the vertical displacements of the region.

1.5.2 Initial state of the geosphere

The initial state of the SFR repository is defined as the state when the repository is closed and saturated. This is the starting point, in time, for the long-term safety assessment which covers the next 100,000 years.

At the end of the operational period, pumping of groundwater to keep the repository drained will stop. The groundwater will gradually saturate the fractures and pores of the rock adjacent to the repository until full saturation is reached. The groundwater will then continue to fill void spaces in drifts and vaults of the repository, gradually saturating the different construction materials and waste packages present in the repository.

The groundwater pressure will be determined by the regional/local flow in the rock (see further description in Chapter 3) and the hydraulic conductivities and the dimensions of the different structures in the repository (see further the **Barrier process report)**.

1.5.3 Evolution of the geosphere considering process interaction

In order to cover the uncertainty in future climate development, four possible future climate developments for Forsmark, or climate cases, are described and analysed in SR-PSU (see the **Climate report**). The climate evolution in the climate cases is described as a time series of climate domains. The climate domains identified are the temperate-, periglacial and glacial climate domains, which are defined and described in detail in the **Climate report**.

The main safety assessment scenario is based on two climate cases, the *global warming* and the *early periglacial* climate cases. The *global warming climate case* consists of an initial period of 50,000 years with temperate climate domain in Forsmark, followed by a 50,000 year period of alternating periglacial and temperate climate domain. The succession of climate domains in the *early periglacial climate case* is identical to the *global warming climate case*, except for a period of periglacial climate domain around 17,000 years after present. In addition to these cases included in the main safety assessment scenario, the *extended global warming climate case* describes a development where the climate in Forsmark is fully dominated by temperate conditions over the coming 100,000 years. This climate case represents a situation where the concentration of atmospheric CO_2 remains high for a longer period of time than in the *global warming climate case*. These three climate cases include periods of temperate and periglacial climate domain, whereas the glacial climate domain does not occur during the 100,000 year assessment period. The glacial climate domain is however included in the *Weichselian glacial cycle climate case*, which represents a development fully dominated by natural climate variability, as described by repeating conditions reconstructed for the last glacial cycle.

The timing of the first future period of permafrost and freezing conditions at the SFR location is of interest in SR-PSU (**Climate report**), whereas the maximum freezing depth is not. The repository concept (barrier material, repository depth etc) and total assessment time (100 ka or 1 Ma) means that the questions to be answered, and the climate cases built to answer them, need to be different between e.g. SR-Site and SR-PSU (**Climate report**). The earliest occurrence of permafrost and frozen ground at the SFR location occurs around 17,000 years after present in the *early periglacial climate case*. During this period, bedrock temperatures below 0°C cannot be ruled out at SFR depth (see the **Climate report** and Brandefelt et al. 2013).

Current scientific knowledge on future climate evolution, reviewed in Section 3.3 of the **Climate report**, suggests that the combination of human intervention and relatively small-amplitude variations in insolation will lead to a global climate evolution in the next 100,000 years which is significantly different from previous glacial cycles. Therefore, the *Weichselian glacial cycle climate case* is not suitable for the analysis of e.g. timing of the first future freezing of SFR. Instead, it has been included in the safety assessment in order to cover remaining uncertainties regarding the presence of an ice sheet during the next 100 ka *and* also as point of reference for the other climate cases.

The impact of ice sheet development in Forsmark is covered by a residual safety assessment scenario that assumes completely degraded concrete barriers and no geosphere retention (**Main report**, Chapter 7). For this safety assessment scenario, detailed information on the geosphere retention process relevant in the glacial climate domain is hence treated pessimistically. In this report, however, some of the geosphere processes relevant in the glacial climate domain are described for completeness. Some other processes, such as deformation of intact rock, are not considered based on the above mentioned pessimistic assumption in the scenario of completely degraded concrete barriers.

1.5.4 Site specific information

The SR-PSU assessment is based on site-specific data and site-descriptive models of the SFR area (SKB 2013b). In some cases, e.g. the 2D permafrost modelling performed by Brandefelt et al. (2013), geosphere data obtained from earlier site-descriptive model versions was used. The final result of the quantitative evaluations of the processes in the different scenarios analysed in SR-PSU will, in many cases, be relying on site-specific data or modelled data, reported in dedicated model studies for the support of the safety analysis (e.g. Odén et al. 2014). In addition, the most essential data for the safety assessment calculation and modelling are thoroughly described in the **Input data report** and the **Data report**.

1.5.5 Time periods of the assessment and reference evolution SR-PSU

The SR-PSU reference evolution includes periods of temperate and periglacial climate domain (**Climate report**, Section 1.3). The main scenario in SR-PSU covers an assessment period of about 100,000 years, which is similar to the duration of a Late Pleistocene glacial cycle (**Climate report**). The main scenario does not cover the excavation and operational period of the repository. However, since this period influences the initial state of the system, it is addressed in some chapters of this report. Process interactions are mainly analysed for periods of temperate or periglacial climate domain. Glacial climate conditions are discussed for some processes, such as methane hydrates, which are only relevant in relation to the occurrence of this climate domain. Based on current scientific knowledge, as described in Section 1.5.3 and in the **Climate report**, the glacial domain is not included in the reference evolution.

In order to reflect different conditions of relevance for repository performance during the assessment period, the following time periods are addressed in the descriptions of the handling of the processes: excavation/operation period, temperate period, periglacial climate and glacial climate conditions (if relevant for the process).

1.6 Headings used when describing each process in this report

All the processes are sorted following a "THMC" thematic approach consisting of thermal, hydraulic, mechanical and chemical processes. The last section, describing transport issues, connects well to the overall radionuclide transport modelling (**Radionuclide transport report**).

1.6.1 Information within each process description

Overview/general description

Under this heading, a general description of the knowledge regarding the process is given. The focus of the description is to support the selected handling in SR-PSU and the handling of uncertainties that are documented under separate headings.

Dependencies between process and geosphere variables

For each system component, in this case the geosphere system, a set of physical variables that define the state of the system is specified (see Section 1.4.2). 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-PSU is indicated in the table.

Boundary conditions

The boundary conditions for each process are discussed. The boundary here refers to the boundary of the geosphere system (see Section 1.4.2). The processes for which boundary conditions need to be described are, in general, related to transport of materials or energy across the boundaries. For example, the discussion of boundary conditions for chemical processes occurring in the geosphere is in general related to the boundary conditions of the relevant transport processes occurring in the geosphere, i.e. advection and diffusion.

Model studies/experimental studies

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

Natural analogues/observations in nature

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

Time perspective

The time scale or time scales on which the process occurs is documented, if such timescales can be defined. If they cannot be defined, this is stated.

Handling in the safety assessment SR-PSU

Under this heading, the handling of the process in SR-PSU is described. Typically, the process is either neglected on the basis of the information under previous headings, or included by means of modelling.

Different aspects are considered when deciding upon a method handling a certain process:

- Time periods over which the process is relevant for system evolution.
- Handling of boundary conditions.
- Handling of the interactions between variables and the process.
- Handling of couplings to other processes.

Handling of uncertainties in SR-PSU

Under this heading, different types of uncertainties associated with the selected handling of the process in SR-PSU are described. These uncertainties are described under the following subheadings.

Uncertainties in mechanistic understanding

The uncertainty in the general understanding of the process is discussed based on the preceding documentation and with the aim of answering the question: Are the basic scientific mechanisms behind the process understood?

Model simplification uncertainty

In most cases, the quantitative representation of a process will contain simplifications. These may result in a significant source of uncertainty in the description of the system evolution. Alternative models or alternative approaches to simplification for a particular conceptual model may sometimes be used to illustrate this type of uncertainty.

Input data and data uncertainty

The set of input data necessary to quantify the process is documented. The further treatment of important input data and input data uncertainties is described in the **Data report,** to which reference is made if relevant.

Adequacy of the references supporting the handling in SR-PSU

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

References

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

1.7 Participating experts

The experts involved in assembling the basic information on the geosphere processes in SR-PSU, and in SR-Site, are listed in Table 1-3. In many cases the same expert has been engaged in SR-PSU as in SR-Site. In those cases, when new experts have been engaged, the SR-Site expert has given comment and corrections to the text. Each section has thereafter been modified to a greater or lesser extent, for the specific needs of the SFR repository and SR-PSU safety assessment. The introductory part of this report has been compiled with input of the SR-PSU team. For each of the sections of Chapters 2 to 6 in this report, the subsections "Handling in safety assessment", "Uncertainties" and "Adequacy of supporting references" have been either formulated by members of the SR-PSU team or by experts in the subject area. The SR-PSU expert of the respective section has been given the chance to comment on the text of these subsections, but the final acceptance of the handling and content of these above mentioned subsections, is that of the SR-PSU team. Final editorial support provided by Jenny Brandefelt is greatly acknowledged. The team's work with the **Geosphere process report** has been led by Teresita Morales, SKB and Martin Löfgren, Niressa.

Table 1-3. Experts responsible for writing the process documentation or responsible for the subject area within SR-PSU and/or in SR-Site. All organisations are based in Sweden, unless explicitly stated.

Process		SR-PSU expert Author, affiliation	SR-Site expert
2.1	Heat Transport	Jens-Ove Näslund, SKB; Martin Löfgren, Niressa	Harald Hökmark, Clay Technology
2.2	Freezing	Jens-Ove Näslund, SKB	Jens-Ove Näslund, SKB
3.1–2	Groundwater flow	Magnus Odén, SKB; Sven Follin,	Jan-Olof Seelroos, SKB
3.3	Gas flow/dissolution	Ivars Neretnieks; Luis Moreno, Royal Institute of Technology	Jan-Olof Selroos, SKB
4.2	Deformation of intact rock	Eva Hakami, Geosigma	Harald Hökmark, Clay Technology
4.3	Displacement along existing fractures	Eva Hakami, Geosigma	Harald Hökmark, Clay Technology
4.4	Fracturing	Eva Hakami, Geosigma	Harald Hökmark, Clay Technology
4.5	Erosion and sedimentation in fractures	Eva Hakami, Geosigma	Harald Hökmark, Clay Technology
5.2*	Advective transport/mixing of dissolved species	Magnus Sidborn, Kemakta	Maria Gimeno, University of Zaragoza, Spain. Ignasi Puigdomench
5.3	Diffusive transport in the rock mass	Martin Löfgren, Niressa	Kristina Skagius, Ignasi Puigdomech, SKB
5.4*	Speciation and sorption	James Crawford, Kemakta	Ignasi Puigdomenech,
5.5	Reactions groundwater/ rock matrix	Björn Sandström, WSP,	Eva-Lena Tullborg, Geologica
5.6	Dissolution/precipitation of fracture-filling minerals	Björn Sandström, WSP,	Eva-Lena Tullborg, Geologica
5.7*	Microbial processes	Miranda Kieth-Roach, Kemakta	Karsten Pedersen, Microbial analytics; Birgitta Kalinowski, SKB
5.8	Degradation of grout	Magnus Sidborn, Miranda Kieth-Roach, Kemakta	Ignasi Puigdomenech, SKB, Jorge Molinero, Amphos, Spain
5.9	Colloidal processes	Magnus Sidborn, Miranda Kieth-Roach, Kemakta	Susanna Wold, Royal Institute of Technology
5.10	Methane hydrate formation	Martin Löfgren, Niressa	John Smellie, Conterra
5.11	Salt exclusion	Martin Löfgren, Niressa; Jens-Ove Näslund, SKB	John Smellie, Conterra
5.12*	Earth currents	Martin Löfgren, Niressa	Johan Andersson, SKB
6.1	Speciation of radionuclides	James Crawford, Kemakta	Maria Lindgren, Kemakta
6.2	Transport of radionuclides in the water phase	James Crawford, Kemakta	Jan-Olof Selroos, SKB
6.3	Transport of radionuclides in the gas phase	Ivars Neretnieks; Luis Moreno, Royal Institute of Technology	Jan-Olof Selroos, SKB

*) The process has been completely rewritten in SR-PSU.

2 Thermal processes

2.1 Heat transport

2.1.1 Overview/general description

Heat transport, that is transport of thermal energy between two points of differing temperature, can take place by conduction, convection (flow), and radiation (e.g. Bird et al. 1960). Heat can also be transmitted between different phases in conjunction with condensation and evaporation, as well in conjunction with freezing and melting. The issue of freezing and melting is not dealt with in this present section but in Section 2.2. In principle heat can also be transported in conjunction with sublimation, but that is of little interest for the SFR repository. Evaporation and condensation are also of limited interest in the fully saturated geosphere, although it may be of interest for other parts of the repository system. Chemical reactions also consume or produce thermal energy. However, in the geosphere the rate and/or magnitude of such reactions are generally too small to affect the bedrock thermal state. Radioactive decay in the Earth's crust and interior affects the large scale thermal state of the geosphere, but decay in the (local) host rock should be insignificant for the rock temperature.

For determining the temperature evolution in the bedrock, heat transport in the geosphere can more or less be equated to heat transport in the rock matrix by conduction. In principle, heat is also transported by groundwater flowing in fractures, and to an insignificant amount by gas flows. In flowing water, convection is the main heat transport mechanism. However, crystalline rock generally has a low permeability, which means that for the bulk of the rock volume, heat transport by convection is dwarfed by conduction in the rock mass. Concerning the overall bedrock temperature, it can easily be shown that the low flow rates in the rock together with the low mean porosity make the contribution of convection negligible (see e.g. Thunvik and Braester 1980). However, if the temperature in the fracture system is in focus, for example in assessing the local permafrost distribution (see Section 2.2), heat transport by water flow may need to be taken into account. It may be that there are local deviations in the temperature at major fracture zones of the relatively shallow SFR host rock, compared to the overall bedrock temperature.

Under steady-state (time-independent) conditions, the heat transport in solid phases is determined solely by the thermal conductivity λ (W/(m·K)) 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 (J/(m^3·K)), and the density, ρ (kg/m^3). In general, temperature propagation in solids can be designated as a diffusion process with the diffusion constant α (m^2/s), also called thermal diffusivity (see Equation 2-1), which can be obtained by:

$$\alpha = \frac{\lambda}{C \cdot \rho} \qquad \text{Equation 2-1}$$

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. 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 geohermal gradient. The latter provides a measure of the variation of the temperature with depth. At a depth of 500 m, the temperature is between 5.5°C and 14.5°C in Swedish bedrock (Ahlbom et al. 1995). Presently at the Forsmark site, the in situ temperature is around 12°C at 500 m depth with a thermal gradient of 11–13°C/km (SKB 2010b, Section 6.2.10). Near the ground surface and down to a depth of several hundred metres there is a climatic impact on the temperatures and temperature gradients. This is of great concern for the SFR repository and the fluctuating temperature of the host rock is described in the **Climate report** and also, as associated with freezing, in Section 2.2. Presently the temperature at the SFR site is about 7°C from about ten metres depth to a few hundred metres depth (e.g. Väisäsvaara 2009, Appendix KFR105.2.3). This temperature, plus minus one or two degrees, is also representative for the Forsmark site investigation area (for the KBS-3 repository) at a similar depth (SKB 2008d, Figure 6-5). As the SFR site emerges from the Baltic Sea, the temperature situation is expected to equal that of the Forsmark site investigation area. Heat generated by radioactive decay in the SFR waste is small (see the **Waste process report**, Section 3.1.2) and can be disregarded for all practical purposes when evaluating the temperature in the geosphere. In addition, heat is created by chemical reactions in conjunction with corrosion and concrete degradation in the repository. In the long term, the effect on the host rock temperature is minor and can be disregarded. The exception is perhaps for the very initial phase after repository closure. This initial impact on the host rock temperature is of little significance for repository safety, as the rock temperature is of the greatest concern during the periglacial climate domain; that is many thousands to tens of thousands of years after repository closure. In summary, one can expect that the temperature of the SFR host rock varies from ~10°C down to a few degrees minus during the assessment time frame.

The bedrock temperature is of consequence for most of the processes described in this report. For example, the temperature affects hydrodynamic properties and the phase state of water, as well as equilibration constants and the kinetics of reactions. As can be seen in the standardised influence tables (e.g. Table 6-1), "temperature in bedrock" is a geosphere variable. Therefore, for each of the discussed processes there is a very short description of how the temperature affects the process, and how the process affects the temperature. Not to preempt the discussions in the following sections, interactions between temperature and other processes are not generally discussed in detail in this present section.

2.1.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 2-1 outlines how the process is influenced by the defined geosphere variables, while Table 2-2 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event the described influence is valid. The nature of the influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is a brief description of the handling of the influence in the safety assessment SR-PSU. In Section 2.1.7, this handling is discussed.

Table 2-1. Direct influences of defined geosphere variables on the process "heat transport" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 2.1.7)
Temperature in bedrock	Yes. Temperature gradients drive heat transport.	All	Heat transport by conduction is included in permafrost modelling.
Groundwater flow	Yes. Heat transport occurs through convection.	All	Heat transport by convection is included in permafrost modelling.
Groundwater pressure	No.	All	–
Gas phase flow	Yes. Heat transport occurs through convection.	All	Negligible amount of heat is transported. Neglected in SR-PSU.
Repository geometry	Yes. As heat is produced in the repository.	All	Heat production in the repository is small and therefor neglected in permafrost modelling.
Fracture and pore geometry	No, but indirectly through: Groundwater flow.	All	–
Rock stresses	No.	All	–
Matrix minerals	Yes. Determines thermal properties and radiogenic heat production.	All	Site specific values of mineral thermal properties are used in modelling. Radiogenic heat production in (local) host rock is neglected.
Fracture minerals	Yes. Marginally and locally by fracture mineral conduction.	All	Neglected in SR-PSU, see text for justification.
Groundwater composition	Yes. If this causes exothermal or endothermal reactions.	All	Neglected in SR-PSU, see text for justification.
Gas composition	Yes. If this causes exothermal or endothermal reactions.	All	Neglected in SR-PSU, see text for justification.
Structural and stray materials	Yes. If degradation of such material creates (or requires) heat.	All	Neglected in SR-PSU, see text for justification.
Saturation	No, but indirectly through: Groundwater flow, in case of partly saturated fracture system.	All	–

Explanation of Table 2-1

Temperature in bedrock

Temperature differences between different points in space comprise the driving force for heat transport. The thermal conductivity and heat capacity of rock are both slightly temperature dependent. For the Forsmark and Laxemar rock types, the conductivity decreases by about 10% per 100°C (Back et al. 2007, Sundberg et al. 2008). The heat capacity of crystalline rock increases typically in 25% per 100°C temperature gradient (SKB 2010c, Table 6-23).

Groundwater flow

The groundwater flow contributes to the heat transport by convection, but because of the low permeability and the low flow rates, this contribution is generally sufficiently small to be ignored in comparison with the conductive heat transport (Thunvik and Braester 1980). However, within the fracture system, and for the rock directly adjacent to the fracture system, flowing water may cause local temperature differences.

Groundwater pressure

The groundwater pressure has no direct influence on the heat transport. However, the groundwater pressure affects the freezing temperature of water, which indirectly affects the heat transport in conjunction to the point in time when such freezing occurs.

Gas phase flow

Only a very small amount of thermal energy can be carried by a gas flow, unless there is a chemical reaction. Accordingly, the influence of (a non-reacting) gas flow on heat transport in the geosphere is negligible. Even if the gas flow is part of a chemical reaction this has very localised thermal effect.

Repository geometry

As the waste produces very small amounts of heat from decay, and as corrosion and degradation in the repository create limited amounts of heat in the long term perspective, the repository geometry is of little consequence for the heat transport in the bedrock. This is especially true thousands or tens or thousands of years after repository closure, at times when there may be permafrost. At early times after repository closure, reactions may affect the temperature of the rock volume adjacent to the rock vaults, but not to the same extent as for a repository for spent nuclear fuel.

Fracture and pore geometry

Fracture geometry affects the groundwater flow. Accordingly, it indirectly affects the local heat flow. The presence of fractures reduces the thermal conductivity, particularly if the fractures are filled with air ($\lambda \approx 0.025$ W/(m·K)) at unsaturated conditions. However, air- or gas-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). This is a two orders of magnitude increase, however the low porosity means that this influence can be neglected. The micropore geometry of the rock matrix is relatively constant in the perspective of heat transport, and has no significant influence on the rock thermal conductivity or heat capacity. In SR-Site, the porosity of the microporous system was estimated to be 0.18% (SKB 2010c, Table 6-90). The volume of the microporous system is expected to typically exceed that of water-filled fractures at the SFR site, if averaged over a larger rock volume, as is indirectly demonstrated in Löfgren (2014).

Rock stresses

Rock stressses have an influence on thermal conductivity, but the effect is small and can be neglected.

Matrix minerals

The thermal conductivity and specific heat capacity of the rock minerals directly affect heat transport (see Section 2.1.1). Also, radioactive decay of naturally occurring nuclides in the much greater rock volume surrounding the SFR repository influences the heat transport.

Fracture minerals

The volumetric ratio of fracture minerals to matrix minerals is very low. Therefore, heat conducted in fracture minerals has little effect on the bedrock temperature. Very locally, the thermal conductivity and specific heat capacity of the fracture minerals may have a minor influence on the heat transport. However, in practice this can be neglected.

Groundwater composition

As the volumetric ratio between water and minerals is so low, the thermal properties of the water are of little consequence for the bedrock temperature. In any case, the groundwater composition is bounded in a very narrow range from the perspective of thermal properties (i.e. thermal conductivity and specific heat capacity). Chemical reactions, caused by non-equilibrium in the groundwater or water/rock interactions, also require or produce thermal energy. However, in the geosphere the rate and/or magnitude of such reactions are generally too small to affect the bedrock thermal state. This should also apply for microbial reactions. When the groundwater freezes or melts, enough energy may be produced or consumed to have a significant impact on the heat transport (see Section 2.2).

Gas composition

As a non-reacting gas flow only can carry insignificant amounts of thermal energy, the composition of such a gas is of no concern. Reactions in the gas phase may create or require heat. However, such reactions are not expected to occur at significant rates in the geosphere.

Structural and stray materials

The volumes occupied by structural and stray materials are too small to influence the heat transport by conduction. In case of corrosion and degradation of such materials, mainly by exothermal reactions, heat is produced. In the SFR host rock the amount of structural and stray materials (rock reinforcements and grouting) is very small compared to that in the waste and engineered components in the rock vaults.

Saturation

The degree of saturation, during the excavation, operation, and the phase of re-saturation of the rock, may affect the groundwater flow (and gas flow) and thus indirectly the heat transport. Also, as discussed under “Fracture and pore geometry”, the presence of unsaturated fractures reduces heat conduction as compared to water filled fractured.

Explanation of Table 2-2

Temperature in bedrock

Heat transport affects the temperature in all parts of the geosphere. The temperature may be altered by heat transport, or be kept at steady state as sustained by heat transport, which predominantly occurs by conduction in the rock matrix.

Groundwater flow

Heat transport will give rise to temperature gradients and density changes of the groundwater that affect large-scale circulatory water movements by so-called density driven flow (see Section 3.2) However, in the shallow host rock surrounding SFR, the effect of density gradients on the groundwater flow is small, compared to the effects of topography related driving forces.

Table 2-2. Direct influences of the process "heat transport" on the defined geosphere variables, and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 2.1.7)
Temperature in bedrock	Yes. Heat transport affects the temperature.	All	Heat transport is included in permafrost modelling.
Groundwater flow	No, but indirectly through: Temperature, which affects density driven flow.	All	–
Groundwater pressure	No, but indirectly through: Temperature.	All	–
Gas phase flow	No, but indirectly through: Temperature and gas composition, affecting for example degassing.	All	–
Repository geometry	No, but indirectly through: Rock stresses, if affecting cave-ins.	All	–
Fracture and pore geometry	No, but indirectly through: Temperature, affecting mineral thermal expansion.	All	–
Rock stresses	No, but indirectly through: Temperature.	All	–
Matrix minerals	No but indirectly through: Temperature.	All	–
Fracture minerals	No, but indirectly through: Temperature.	All	–
Groundwater composition	Yes. Heat transport affects chemical reactions and processes such as salt exclusion.	All	It is generally assumed that heat transport is not a limiting factor when estimating reactions that alter the groundwater composition. Salt exclusion is discussed in Section 5.11.
Gas composition	Yes. For example, degassing requires heat transport.	All	It is generally assumed that heat transport is not a limiting factor when estimating e.g. degassing and reactions altering the gas composition.
Structural and stray materials	Yes. Corrosion and degradation of these materials require heat transport.	All	The away transport of heat released by corrosion and degradation of these materials is assumed not to be limiting.
Saturation	Yes. At excavation and operation, heat from ventilation dries out rock adjacent to tunnels.	E/O/S	The re-saturation phase of the host rock is not modelled in SR-PSU, but is assumed to be quick.
		T,P,G,EQ	Heat transport has no impact on saturation during these periods.

Groundwater pressure

Heat transport will influence the groundwater temperature which, in turn, will influence the groundwater pressure 1) in case of a closed or poorly connected system or 2) to a very minor degree in case of an open system but where the water density slightly changes. In contrast to the conditions in argillaceous rocks, the hydraulic conductivity of crystalline rocks will be sufficient to dissipate thermally induced increases in pore pressure. Selvadurai and Nguyen (1997), for instance, showed that the thermally-induced fluid pressure around a repository located 1,000 m below ground surface, with a significantly higher thermal load than the KBS-3 repository at Forsmark and with a hydraulic conductivity of $1 \cdot 10^{-11}$ m/s at all depths, was only about 2 MPa. Between the SFR repository and the ground surface at Forsmark, the large-scale hydraulic conductivity is orders of magnitude higher and the distance to the ground surface is much less than the repository considered in the model analysed by Selvadurai and Nguyen (1997). This means that any thermally induced fluid pressure deviations in the SFR host rock will be much lower and can be ignored.

Gas phase flow

Heat transport may both affect the gas temperature, and thus its volume, and the degree of gas dissolution and degassing. This may in turn affect a potential gas flow (see Section 3.3).

Repository geometry

Heat transport may affect the rock temperature, and thus the stress state and the degradation rate of rock support. Therefore, the repository geometry may be indirectly altered by cave-ins or rock fallout if such occurs. However, this chain of processes would require greater changes in temperature than is reasonable to assume. No cave-in or fallout is expected to occur at SFR to the degree that the repository geometry would be significantly changed (see Section 4.3).

Fracture and pore geometry

Changes in temperature will to some extent affect the fracture and pore geometry by means of thermal expansion and contraction of minerals. However, the expected temperature range in the host rock is small. Accordingly the effect can be neglected. Effects on the fracture and pore geometry in conjunction to freezing is discussed in Section 2.2 and Chapter 4.

Rock stresses

Heat transport is important for the way thermal stresses are induced. Thermal expansion and contraction of minerals, associated with a change in temperature, will affect the stress state.

Matrix minerals

Heat transport in the relevant temperature range will not influence the overall mineral composition of the rock matrix but may, to a minor extent, lead to mineral dissolution, alteration, and precipitation. Variations in the temperature will very slightly affect the mechanical properties of matrix minerals. This effect can be neglected in the relevant temperature range (see Chapter 4). Also the thermal properties of the matrix minerals can slightly change.

Fracture minerals

Heat transport and subsequent temperature variations may to a minor extent affect the dissolution, alteration, and precipitation of fracture minerals (see Section 5.6).

Groundwater composition

Heat transport is required to sustain endothermal and exothermal reactions in the groundwater, as well as degassing, dissolution, and precipitation. Generally, these processes are thought to be limited by mass transport or kinetics at the ambient temperature, and heat transport in the bedrock is not considered to be limiting (i.e. the reactions will not change the ambient temperature). Large-scale heat transport giving rise to changes in the ambient temperature would shift the equilibrium of the reactions, and thus influence the groundwater composition in an indirect manner. If the heat transport gives rise to freezing, salt exclusion may occur as is further discussed in Section 5.11.

Gas composition

Heat transport is required for degassing and dissolving gasses. Heat transport is also required to sustain endothermal and exothermal reactions in the gas phase, although such reactions are not expected in the geosphere at significant rates. Generally, these processes are thought to be limited by mass transport or kinetics at the ambient temperature, and heat transport in the bedrock is not considered to be limiting (i.e. the reactions will not change the ambient temperature). Large-scale heat transport giving rise to chances in the ambient temperature would shift the equilibrium of the reactions, and thus influence the gas composition in an indirect manner.

Structural and stray materials

The corrosion and degradation of rock support and grouting require that heat transport occurs, as most reactions do. However, this heat transport should not be limiting for the corrosion or degradation rate.

Saturation

During open tunnel conditions, the heat induced into the rock mass by ventilation will dry out a thin layer of the rock mass directly adjacent to the underground openings. Upon closure, fully saturated conditions are assumed to be quickly established and remain regardless of the magnitude of heat transport, within reasonable bounds.

2.1.3 Boundary conditions

Prevailing and past climatic conditions, the geothermal heat flow including radiogenic heat production, and the thermal properties of the rock determine the initial and evolving temperature, temperature gradients, and heat transport.

The ground surface acts as a low temperature boundary, contributing to reducing the temperatures in the repository host rock. The repository/host rock interface creates another boundary. This is partly because there will be minor heat production in the repository, due to both radioactive decay and chemical reactions. Another reason is that the thermal properties of the engineered repository materials (waste, concrete barriers, backfill, etc.) in terms of thermal conductivity and heat capacity differ from those of the host rock. This is definitely the case at unsaturated conditions but also as the repository becomes saturated.

The interface between flowing water and the rock matrix; or the boundary between a frozen flow path and flowing water may exemplify local boundaries within the host rock, over which heat transport takes place.

2.1.4 Model studies/experimental studies

In this section, only studies on the geothermal evolution of the site are discussed, and not studies on the impact of heat transport on other geosphere variables. When deemed appropriate, such studies are discussed in the subsequent chapters.

Given different climate evolutions and surface conditions, heat transport in bedrock has been simulated in 2D for the Forsmark site (Hartikainen et al. 2010). The model domain in these simulations covered both the planned repository for spent nuclear fuel and the SFR repository. In addition, heat transport and bedrock temperatures have been simulated for periods of potential future periglacial climate conditions at Forsmark (Brandefelt et al. 2013). The latter study was specifically designed to assess the risk for permafrost and freezing of the SFR repository structures.

2.1.5 Natural analogues/observations in nature

In this section, only natural analogues and observations in nature that are relevant for the understanding of the geothermal evolution of the site are discussed. Natural analogues and observations relating to the impact of heat transport on other geosphere variables are discussed in the subsequent chapters, when deemed appropriate.

Heat flow estimates for Scandinavia and the Kola Peninsula have been made from observations of drill hole thermal gradients (e.g. Eriksson and Malmqvist 1979, Balling 1995, Mottaghy et al. 2005, Kukkonen et al. 2011). The results show that the Baltic shield has low to moderate heat flow, in general around 40 to 60 mW/m^2. A detailed distributed data set on geothermal heat flux over Sweden and Finland (Näslund et al. 2005), estimated from calculations of e.g. crustal heat production, shows that regional and local variations in geology increase this range to be from 30 to more than 80 mW/m^2. Also at the Forsmark site, the geothermal heat flux has been calculated from observations of bedrock temperature profiles (Sundberg et al. 2009). The palaeoclimatically corrected surface mean heat flow at Forsmark is 56 mW/m^2, with a total uncertainty of +12 to –14%.

2.1.6 Time perspective

The magnitude of heat transport, as well as the bedrock temperature, will progress through repository evolution as the climate evolves. In terms of consequences for the assessed risk, there will likely be times of low temperature during the periglacial climate domain that are of greatest importance. The reason is that low temperatures leading to freezing may be consequential for barrier degradation (see the **Barrier process report**). The first period of the periglacial climate domain is not expected for a long time (tens of thousands of years according to the **Climate report**).

During the initial period after closure, the quickest changes of temperature in rock close to the vaults are likely to occur. However, this will not lead to freezing and, therefore, this period is of limited importance for repository safety.

2.1.7 Handling in safety assessment

In this section, the SR-PSU team gives recommendations on how to handle the process of heat transport, but mainly from the perspective of changing the bedrock ambient temperature. Changes in the bedrock temperature will in turn affect other processes discussed in this report, as described in the corresponding sections. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of the Tables 2-1 and 2-2 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

During this period, the temperature of the rock mass adjacent to the rock vaults differs from that of the surrounding host rock. Even so, the differences are relatively small and should be equalised rather quickly upon repository re-saturation. Heat production from initial corrosion and concrete degradation reactions in the repository may lead to remaining differences in the temperature of the adjacent rock, compared to the larger rock mass surrounding the repository. However, such effects are neglected in SR-PSU as the increased rock temperature is judged to have an insignificant (or at least not a detrimental) impact on repository safety.

Periods of the temperate climate domain

During this period, the temperature of the SFR host rock is assumed to stay within a limited range corresponding to the present situation. No detailed modelling of the temperature's spatial distribution or temporal evolution is made. Instead it is assumed that the present day in situ temperature, as measured within the SFR and Forsmark site investigations, will represent the entire climate domain. As discussed in Section 2.1.1, the host rock temperature at SFR is measured to be around 7°C, plus minus a few degrees.

Periods of the periglacial climate domain

During periods of the periglacial climate domain the temperature of the bedrock may decrease to such low values that groundwater freezes, even at depth. Modelling the evolution of the bedrock temperature and its impact on freezing is important for assessing the repository safety, as further discussed in Section 2.2.

Periods of the glacial climate domain

The heat flow and temperature of the bedrock is affected by changes in climate and climate-related conditions, for instance by the presence of ice sheets (e.g. Kukkonen and Jõeleht 2003). For simulations of permafrost development at Forsmark under glacial cycles, this has been taken into account by incorporating the effect of simulated basal ice temperatures during periods of ice sheet coverage (SKB 2010b).

Earthquakes

Earthquakes are assumed not to alter the thermal state of the host rock. Deviations in the host rock temperature, compared to the natural situation prior to the construction of the SFR repository, are assumed not to change the probability of earthquake occurrence. Furthermore, such deviations are assumed not to modify the nature, or effect, of earthquakes, should such events occur.

Handling relative to geosphere variables

Temperature in bedrock

Heat transport and bedrock temperature are closely related, as described in the above text. Therefore, both entities are integrated in the thermal permafrost modelling in SR-PSU (cf. Section 2.2).

Groundwater flow

Changes in the bedrock temperature are neglected in the SR-PSU hydrogeological modelling, as long as there is no freezing. (cf. Section 3.2).

Groundwater pressure

The very minor changes in groundwater pressure, as response to changes in temperature, are neglected in SR-PSU (cf. Section 3.2).

Gas phase flow

No detailed modelling of gas phase flow in the geosphere is performed within SR-PSU. Consequently, the effect of heat transport on gas phase flow is disregarded. Conversely, the effect of gas phase flow on the bedrock temperature is insignificant and accordingly neglected (cf. Section 3.3).

Repository geometry

When modelling the evolution of the repository geometry (i.e. the risk of cave-ins and rock fallout) changes in the rock's temperature are not incorporated (cf. Chapter 4).

Fracture and pore geometry

Changes in fracture and pore geometry, as result of heat transport or changes in temperature, are neglected in SR-PSU (cf. Chapter 4).

Rock stresses

When modelling the evolution of rock stresses, changes in the rock's temperature are not incorporated (cf. Chapter 4).

Matrix minerals

The site specific thermal properties of the rock matrix are included in thermal modelling (i.e. permafrost modelling) in SR-PSU.

Fracture minerals

The possible impact of fracture minerals on heat flow, and vice versa, is neglected in SR-PSU.

Groundwater composition

The general bedrock temperature is included in groundwater composition modelling as a constant (cf. Chapter 5). It is assumed that heat transport is not a limiting factor for reactions to occur.

Gas composition

No gas composition modelling is made for the geosphere in SR-PSU.

Structural and stray materials

When assessing the degradation of structural and stray materials in SR-PSU, a constant reference temperature is assumed (cf. Section 5.8).

Saturation

The re-saturation of the host rock is expected to be quick, upon repository closure, and is not modelled. Consequently, the potential effect of short-lived and localised unsaturated zones on the thermal state of the host rock is neglected in SR-PSU.

2.1.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Heat transfer through the geosphere and across the ground surface is a relatively uncomplicated process, at least if it is assumed that the heat transport occurs by conduction and convection and that no heat is produced of consumed in the local host rock (except for during periglacial periods where freezing and melting of ice is accounted for). The processes described are based on fundamental physical laws without significant conceptual uncertainties. In addition, there is an abundance of empirical observations that support the mechanistic understanding.

Model simplification uncertainties

In SR-PSU, heat transport in conjunction with modelling of perennially frozen grounds is assumed to occur by conduction and convection (2D). Heat transport associated with endothermal and exothermal reactions is neglected, in the context of the host rock's thermal state.

2.1.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

2.2 Freezing

2.2.1 Overview/general description

Permafrost is commonly defined as ground which temperature remains at or below 0°C for at least two years in a row (French 2007), regardless if the ground is frozen or not at this temperature, whereas *perennially frozen ground* is defined as ground that keeps frozen for at least two consecutive years. For further discussion of these and other related definitions of terms, see Dobinski (2011).

Fresh water freezes at a temperature of 0°C under atmospheric pressure. The freezing process is primarily governed by the temperature, but is also affected by i) the prevailing pressure, ii) chemical composition of the water (presence of solutes) and iii) the adsorptive capacity of water in soil and rock. Regarding the pressure influence, freezing of water occurs when temperature and pressure satisfies the generalised Clapeyron equation (e.g. O'Neill and Miller 1985). This results in the melting or freezing temperature being depressed with increasing pressure by 0.08°C/MPa in the pressure range 0.1–50 MPa, as depicted in Figure 2-1a. Just as in the case with an increasing pressure, an increase in solutes in liquid water also depresses the melting/freezing temperature. This is referred to as the osmotic pressure (e.g. Padilla and Villeneuve 1992), shown in Figure 2-1b.

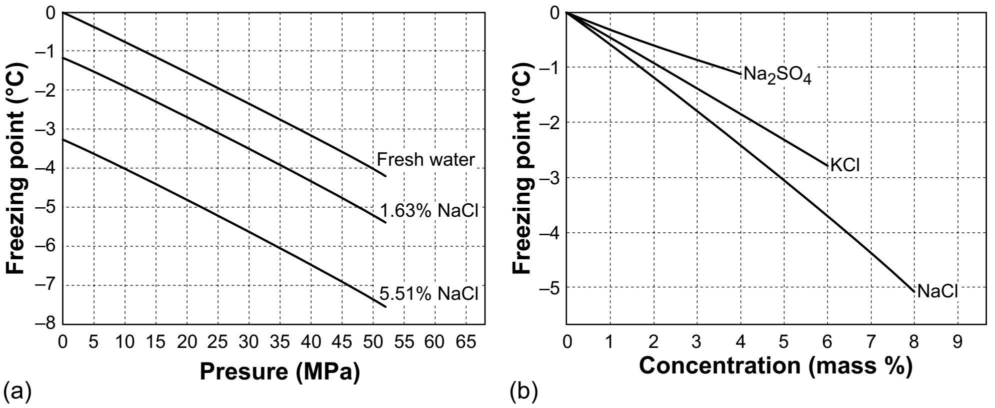

Figure 2-1. *(a) Pressure–freezing point diagrams for fresh water from CRC (1998) and for NaCl aqueous solutions of concentrations of 1.63 and 5.51 weight-% from Guignon et al. (2005). (b) Concentration–temperature phase diagrams at normal atmospheric pressure for NaCl, KCl and* Na_2SO_4 *aqueous solutions from CRC (1998).*

The adsorptive capacity of the geosphere depends mainly on the physical properties and the specific surface area of the minerals. Hence, a larger adsorptive capacity and finer pores in a soil results in a lower freezing temperature of water (Hohmann 1997). This is especially important when ice crystals are growing in small pores, such as within sediments and rock. For example, in clays, liquid water has been observed at temperatures down to –10°C (O'Neill and Miller 1985).

Freezing of groundwater is an integral part of the physical processes occurring in the geosphere under cold climates and has a direct or indirect impact on its thermal, hydrochemical and mechanical behaviour. Heat transfer is influenced through the thermal properties of the geosphere and by latent heat from the phase change.
Since the conduction of heat is the main process that determines heat transfer in the geosphere (e.g. Hartikainen et al. 2010), except in highly conductive fracture zones, the amount of freezing water dominates the rate of freezing and the depth to which freezing can extend. In principle, the larger the amount of freezing water, the lower the freezing rate. This results from the fact that the warming effect due to the latent heat overcomes the cooling effect due to the increased thermal diffusivity in the frozen ground.

Since the thermal regime of the geosphere does not involve any heat sinks that can cool the temperature below 0°C, freezing of the soil and bedrock can only develop from the ground surface and downwards. When freezing migrate downwards, there is a gradual transition from unfrozen conditions to conditions with an increasingly larger content of frozen water. In this way, there is typically, within the permafrost, rock volumes that contain unfrozen water below 0°C, see Figure 2-2. The freezing thus takes place gradually over a vertical freezing zone.

Freezing of groundwater may results in the ground becoming nearly impermeable, which in cases of widespread permafrost strongly reduces the regional groundwater flow and changes the overall groundwater circulation (e.g. Hartikainen et al. 2010, Vidstrand et al. 2010a). Exclusion of salts can occur during the freezing of saline groundwater, leading to a redistribution of the salinity concentration around the freezing zone that migrates downward (Hartikainen et al. 2010, SKB 2010e, 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, Yershov 1998, French 2007).

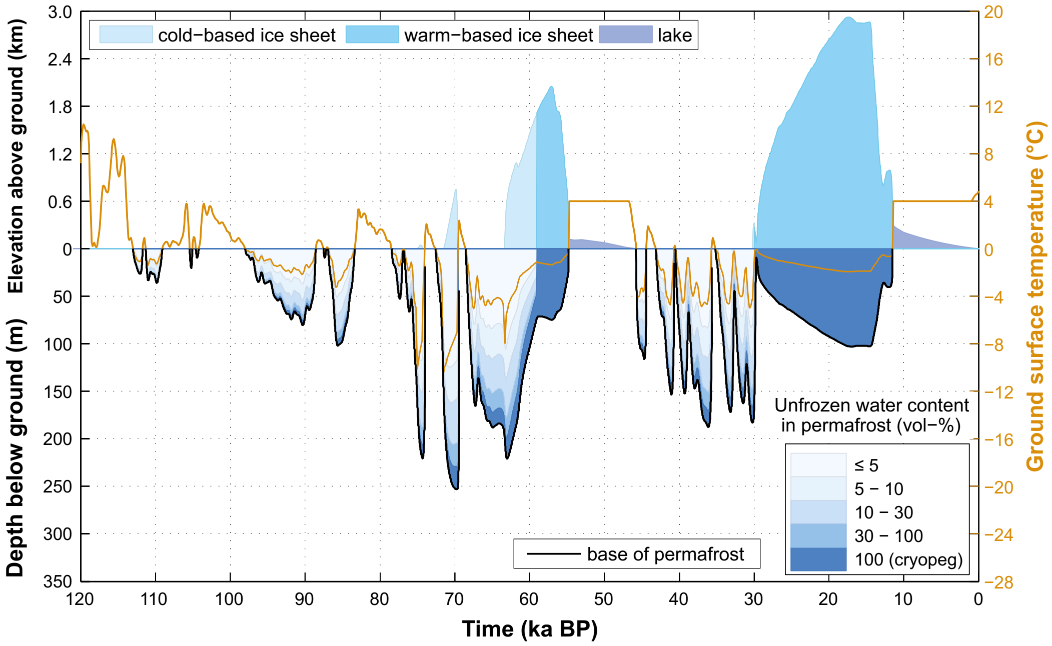

Figure 2-2. Example of unfrozen water content within permafrost for conditions at Forsmark reconstructed for the last glacial cycle. The figure also show surface conditions in terms of ice sheet coverage and submerged conditions. Note that the unfrozen water content may be substantial within large parts of the permafrost, with increasing values towards the permafrost base. For information on the permafrost simulation, see SKB (2010b, Section 3.4.4).

If future cold climate conditions result in an ice sheet reaching the Forsmark site, as exemplified in the Weichselian glacial cycle climate case (**Climate report**), it is highly likely that periglacial climate conditions prevail prior to the glacial period. In line with this, it is expected that the SFR repository typically would be frozen at the time of ice sheet overriding. During the time period when the repository is covered by the ice sheet, permafrost is likely to diminish due to the insulation effect of the overlying ice mass, especially if the ice sheet is warm-based (**Climate report**). It is thus expected that the site in general would not have permafrost and frozen repository conditions at the time of deglaciation. Furthermore, if the site is covered by the Baltic sea after deglaciation, due to the isostatic response to ice sheet loading, permafrost would not be able to form at the repository location during the submerged period.

2.2.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 2-3 outlines how the process is influenced by the defined geosphere variables. Table 2-4 shows how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. In Section 2.2.7, this handling is elaborated upon in a discussion provided by the SR-PSU team.

The nature of the influence between the process and each geosphere variable is elaborated upon below.

Explanation of Table 2-3

Temperature in bedrock

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

Table 2-3. Direct influences of defined geosphere variables on the process "freezing" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 2.2.7)
Temperature in bedrock	Yes.	P/G	Temperature from model calculations of heat transport (Section 2.1).
Groundwater flow	Yes. But mainly in highly conductive fractures with large flow.	P/G	Included in 2D permafrost model.
Groundwater pressure	Yes.	P/G	Included in permafrost model.
Gas phase flow	Yes. But only in highly conductive fractures with large groundwater flow.	P/G	Neglected; little significance.
Repository geometry	No.	P/G	–
Fracture and pore geometry	Yes. The amount of freezing water is related to fracture geometry.	P/G	Continuum porous medium models adopted. Detailed fracture geometry neglected; low-porosity rocks. See further Section 3.2.7 and 3.2.8.
Rock stresses	No. But indirectly through fracture geometry and groundwater pressure.	P/G	–
Matrix minerals	Yes. Through thermal properties, affecting heat transport and temperature.	P/G	Handled in permafrost model.
Fracture minerals	Yes. Affects water adsorption capacity.	P/G	Neglected; little significance compared with other influences.
Groundwater composition	Yes.	P/G	Use of site-specific groundwater salinities in modelling studies.
Gas composition	Yes. But only when vapour–ice phase change occurs.	P/G	Neglected; little significance.
Structural and stray materials	No. But indirectly through their thermal properties and impact on groundwater composition.	P/G	–
Saturation	Yes. Affects the amount of freezing water.	P/G	Neglected; saturated conditions in the bedrock are assumed.

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 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 groundwater pressure decreases the freezing point. In turn, the groundwater pressure is affected by the amount of freezing water in the pore space, the mechanical properties of the geosphere and the effective stress state of the rock.

Gas phase flow

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

Repository geometry

The repository geometry does not have any direct influence on the freezing process.

Fracture and pore geometry

The amount of freezing water and the adsorptive properties of the host rock depend on the fracture geometry. In fractures with varying aperture (in effect all fractures) wider parts may freeze while narrow parts remain unfrozen unless the temperature is lowered further. See further Sections 3.2.7 and 3.2.8.

Freezing can have some influence on the fracture geometry at shallow depths due to frost cracking. Close to the ground surface frost wedges can be formed to the depth of some metres. Otherwise, there can be widening of fractures due to freezing.

Rock stresses

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

Matrix minerals

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 downward propagation of the freezing zone.

Fracture minerals

The adsorptive capacity of the host rock 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 cation exchange reactions between soil mineral particles and adsorbed water (Yershov 1998).

Groundwater composition

The composition of the groundwater affects the freezing point in such a way that the freezing point is decreased with increasing concentration of compounds like dissolved salts. Exclusion of salts during freezing can lead to redistribution of groundwater composition (Hartikainen et al. 2010, SKB 2010e, 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.

Explanation of Table 2-4

Temperature in bedrock

Latent heat is released when freezing of water occurs. This increases the temperature of the surrounding rock.

Groundwater flow

Frozen ground is typically close to impermeable. Groundwater may only flow in adjacent or deeper unfrozen rock volumes. This may result in a drastically different flow pattern. In summertime, water may also flow in the active layer that thaws above the permafrost.

Table 2-4. Direct Influences of the process "freezing" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 2.2.7)
Temperature in bedrock	Yes. Through the release of latent heat in the freezing process.	P/G	Included in permafrost model.
Groundwater flow	Yes.	P/G	Included in 2D permafrost model. See also Section 3.2 Groundwater flow.
Groundwater pressure	Yes. By partial freezing of water in the pore space.	P/G	Included in permafrost model.
Gas phase flow	Yes.	P/G	See Section 3.3 Gas flow/dissolution.
Repository geometry	No.	P/G	–
Fracture and pore geometry	Yes. By volume increase going from liquid to solid state.	P/G	Neglected, little significance.
Rock stresses	No. But indirectly through fracture geometry.	P/G	–
Matrix minerals	No.	P/G	–
Fracture minerals	No.	P/G	–
Groundwater composition	Yes. By exclusion of salt.	P/G	Included in 2D permafrost modelling. See also Sections 5.11 and 3.2.
Gas composition	Yes. But only when vapour ice phase change occurs.	P/G	Neglected; little significance.
Structural and stray materials	Yes. But only if freezing occurs at repository depth.	P/G	Neglected; the resistance due to grouting is not accounted for in the flow modelling, see Section 3.2.
Saturation	Yes. Saturated volume decreases.		Neglected; saturated conditions in the bedrock are assumed.

Groundwater pressure

Permafrost may affect the pressure due to the effects of partial freezing of water in the pore space. Included in the modelling of permafrost.

Gas phase flow

See Section 3.3 (not included in permafrost modelling).

Repository geometry

The geometry is not included in permafrost modelling, however, indirectly dependant on it.

Fracture and pore geometry

Minor influence by volume increase when groundwater going from liquid to solid state, and therefore neglected in SR-PSU.

Rock stresses

There is no major influence on this variable from freezing processes, but indirectly through fracture geometry. This is not included in the modelling of permafrost.

Groundwater composition

Exclusion of salt may occur during the freezing process, which would increase the salinity within or beneath the downward migrating freezing zone. Included in 2D permafrost modelling.

Gas composition

Freezing may have an influence on gas composition, but only if there is a vapour ice phase change. This influence is however thought of having little significance and is neglected.

Structural and stray materials

Structural and stray materials may be affected but only if freezing occurs at repository depth.

Saturation

With time, the saturated volume decreases, however this influence is neglected since saturated conditions in the bedrock are assumed.

2.2.3 Boundary conditions

Thermal boundary conditions

Groundwater freezing requires that the ground surface temperature is below 0°C. The ground surface temperature in turn is the result of heat exchanges across the boundary layers (vegetation-, snow-, and/or soil cover) between the atmosphere and the ground (Washburn 1979, Lunardini 1981, Smith and Riseborough 1996, Yershov 1998). Depending on the climatic conditions and the characteristics of these boundary layers, the inter-annual ground surface temperature can deviate from the air temperature in a range between approximately –1 and +8°C. This may be exemplified by air temperatures and modelled ground surface temperatures for Forsmark (Figure 2-3).

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

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

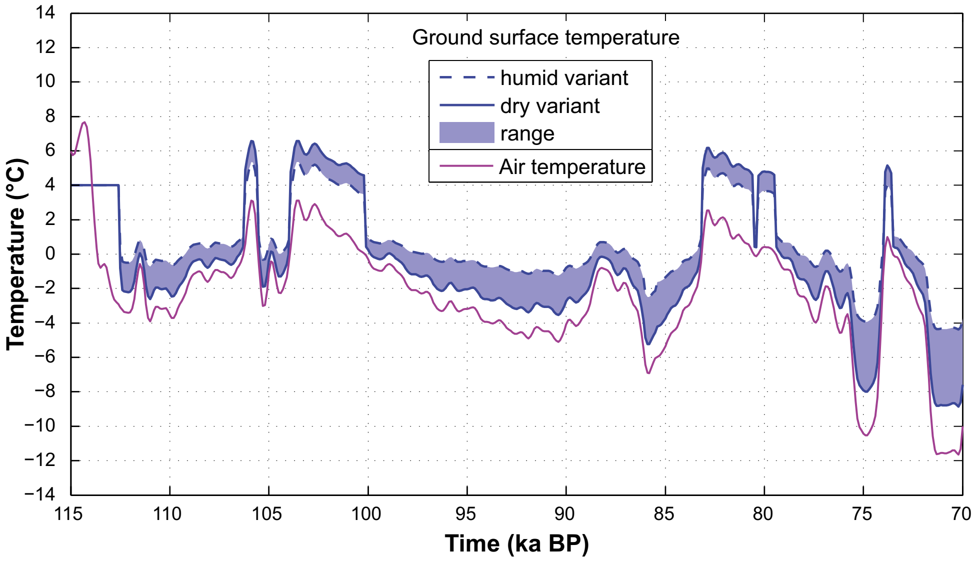

Figure 2-3. *Example of air temperature curve reconstructed for Forsmark for the first c. 45,000 years of the last glacial cycle and associated modelled ground surface temperatures (Hartikainen et al. 2010). The figure shows results extracted for a location above the planned repository for spent nuclear fuel. Calculated ground surface temperatures are shown for one dry and one humid variant of climate development. Note that ground surface temperatures are several degrees warmer than the air temperature. Uncertainties in the air temperature curve are discussed in the SR-Site Climate report (SKB 2010b, Section 3.4.4 and Appendix 1).*

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

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

Hydraulic boundary conditions

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

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

Mechanical boundary conditions

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

2.2.4 Model studies/experimental studies

Relevant issues relating to freezing processes in the geosphere, based on literature reviews, have been reported by e.g. Gascoyne (2000), Ahonen (2001), Vidstrand (2003) and Vidstrand et al. (2010a). Experimental investigations of thermal, hydrochemical and mechanical impacts of freezing on bedrock properties have been reported by Wegmann et al. (1998), Ruskeeniemi et al. (2002, 2004) and Kleinberg and Griffin (2005), whereas model studies dealing with permafrost development in ground under climate change can be found in e.g. Lunardini (1995), Delisle (1998), Kukkonen and Šafanda (2001), Froese at al. (2008), Bense et al. (2009), Hipp et al. (2012), Jafarov et al. (2012) and Brandefelt el al. (2013). Model studies on thermo-hydro-mechanical impacts of freezing processes on bedrock properties with implications for interactions between glaciers and permafrost on orbital timeframes have been conducted, e.g. Bauder et al. (2003), Delisle et al. (2003), Hartikainen (2004), SKB (2006a), Person et al. (2007), Lemieux et al. (2008a, b, c) and Hartikainen et al. (2010). The effects of freezing of the geosphere on groundwater and surface water flow have been studied by e.g. Edmunds (2001), Carlson et al. (2007), Vidstrand et al. (2008, 2010a, b), Boulton et al. (2009), Lyon et al. (2009), Norman and Sykes (2010), Holmén et al. (2011), Bosson et al. (2012), Finney et al. (2012), Walvoord et al. (2012), Grenier et al. (2013), van der Ploeg et al. (2012), Provost et al. (2012) and Selroos et al. (2013).

Simulations of bedrock temperatures and development of permafrost have been performed for SR-PSU in order to assess the earliest potential future period for freezing of the SFR concrete barriers (Brandefelt et al. 2013). Climate model simulations were performed for future periods of low insolation (17 and 54 ka after present) and air temperature data from these periods were used as input to simulations of permafrost and perennially frozen depths. To this end, the same permafrost model and model domain as used in Hartikainen et al. (2010) were used, see Brandefelt et al. (2013).

2.2.5 Natural analogues/observations in nature

Freezing of water in the geosphere is a common feature in Boreal and Arctic climates that occur in the temperate and periglacial climate domains. 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 on glaciers (e.g. Holmlund et al. 1996, Pettersson et al. 2003, Jansson et al. 2000, Gusmeroli et al. 2012) shows that perennially frozen ground exists also beneath glaciers. A full-scale field experiment on the growth of permafrost was conducted by Mackay (1997).

To advance the understanding of processes associated with glaciation and their impact on the long-term safety of geological repositories, the Greenland Analogue Project (GAP), a four-year field and modelling study of the Greenland ice sheet and geosphere conditions, was initiated collaboratively by SKB, Posiva and NWMO. In this study, detailed observations of permafrost characteristics are made, as well as studies of the coupling to bedrock thermal characteristics and hydrogeological- and hydrogeochemical conditions (Harper et al. 2011).

A large number of studies address questions related to permafrost thawing due to climate warming, e.g. Kuhry et al. (2010), Romanovsky et al. (2010a, b) and Vonk et al. (2012), see also Section 2.2.4.

The present-day distribution of permafrost in the Northern Hemisphere is illustrated in Figure 2-4.

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

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

2.2.6 Time perspective relative to SR-PSU

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 and 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 at Forsmark decreases from the present-day value to a value of below approximately –8 to –10°C, perennial freezing of ground can develop down to 400 m depth in the bedrock in a time frame of 100,000 years, as illustrated in Figure 2-5.

2.2.7 Handling in safety assessment

In this section, the SR-PSU team gives recommendations on how to handle the process of freezing. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 2-3 and 2-4 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/resaturation period

Not relevant, since development of perennially frozen ground is not expected during these periods (**Climate report**).

Temperate climate domain

Not relevant, since development of perennially frozen ground per definition does not occur in the temperate climate domain (**Climate report**).

Periglacial climate domain

The *periglacial climate domain* prevails in areas where perennially frozen ground exist, but without the presence of an ice sheet (**Climate report**). The timing of the expected first future periods of cold climate conditions, and the associated potential for development of permafrost and perennially frozen ground at Forsmark and SFR, are investigated by coupled climate- and 2D permafrost modelling (Brandefelt et al. 2013). The climate model simulations consider e.g. the known future variation in insolation and various possibilities of greenhouse gas concentrations.

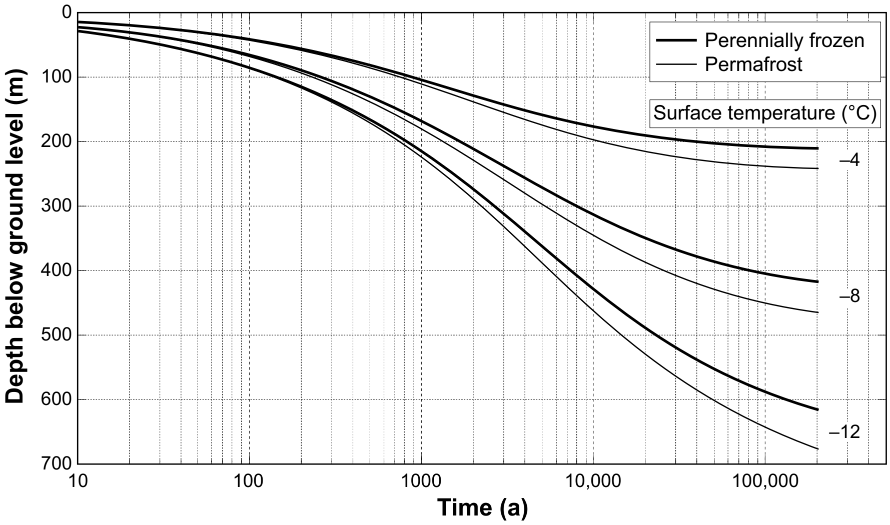

Figure 2-5. *Evolution of permafrost (0°C-isotherm) depth and perennially frozen ground depth for constant ground surface temperatures of –4, –8 and –12°C at the Forsmark site with present-day mean characteristics (after SKB 2010b).*

The permafrost simulations in turn are based on air temperature output from the climate models and site-specific characteristics and initial conditions. This study provides the thermal conditions of the ground for future cold climate periods, summarised in the **Climate report**, which are used for further assessment of the risk for and consequences of freezing of SFR repository structures at different repository depths.

In addition, development of permafrost and the depth of perennially frozen ground together with the evolution of ground temperature during typical glacial cycle conditions, including temperate, periglacial and glacial climate domains (SKB 2010b), are estimated by 1D and 2D permafrost model simulations. For this reconstruction of permafrost development for the last glacial cycle, surface boundary conditions are produced by ice sheet- and global isostatic adjustment modelling.

Glacial climate domain

The *glacial climate domain* prevails wherever the ground is covered by glaciers or ice sheets (**Climate report**). Freezing and thawing of perennially frozen ground overlain by an ice sheet is handled and described in the reference glacial cycle climate case (**Climate report**). This situation is described by 1D permafrost simulations (SKB 2010b).

Earthquakes

Not relevant. On the other hand, there is a possibility to have glacially induced earthquakes, although those are not caused by freezing *per se*.

Handling relative to geosphere variables

Temperature in bedrock

Included in permafrost model.

Groundwater flow

Included in 2D permafrost model. See also Section 3.2 Groundwater flow.

Groundwater pressure

The effects of the pressure induced by partial freezing of water in the pore space is included in the permafrost model.

Groundwater composition

Salt exclusion effects are included in 2D permafrost modelling. See also Sections 5.11 and 3.3.

2.2.8 Handling of uncertainties

Uncertainties in mechanistic understanding

There are no major uncertainties in understanding of mechanistic processes regarding freezing and permafrost development. Minor uncertainties are associated with the fact that the geochemical weathering characteristics of the geosphere due to freezing and thawing processes are not yet well-founded. One process that is well known is that repeated freeze–thaw cycles induce fracturing of rock and lead to a general decrease in the size of the particles produced. As the particles of frost-weathered rock get smaller, their surface area increases and therefore chemical weathering is increased.

Model simplification uncertainties

Permafrost simulations have been performed in 2D and 1D. The 2D study by Brandefelt et al. (2013) was specifically made for answering questions of relevance for SR-PSU. It also constitutes a complement to previous 1D and 2D permafrost studies performed for SR-Site (Hartikainen et al. 2010, SKB 2010b).

The 2D permafrost simulations performed within SR-PSU were conducted in order to investigate the timing and potential for permafrost and perennially frozen ground the coming 60,000 years (Brandefelt et al. 2013). Together with the 2D simulations performed for SR-Site (Hartikainen et al. 2010), they also illustrate the site specific spatial (along the profile) development of permafrost and frozen ground at Forsmark.

The major model simplification in the 2D simulations is the exclusion of a 3D groundwater flux. However, compared with heat conduction, groundwater flow has only a minor role in permafrost development, as indicated by the difference between 2D modelling with a rudimental groundwater flow (Hartikainen et al. 2010) and 1D modelling completely lacking groundwater flow (SKB 2006a, 2010b), see Hartikainen et al. (2010). Furthermore, the anisotropy of thermal properties is not a problem in 1D or 2D, since one can choose a combination of thermal properties that would give the lowest temperatures, or at least very close to the lowest temperatures. Therefore, it is unlikely that 3D simulations would yield notably lower temperatures than the range obtained by the full series of 1D and 2D sensitivity modelling studies that were performed for SR-Site (Hartikainen et al. 2010).

The major model simplification in 1D permafrost modelling studies is the exclusion of lateral variations in physical properties, boundary conditions and geometry. For example, full consideration of the anisotropy of thermal conductivity and heat capacity and the features of water bodies and topography, requires 3D modelling. However, this is to a large extent taken care of by the 2D modelling that has been performed (Hartikainen et al. 2010, Brandefelt et al. 2013). Minor uncertainties in the 1D modelling simulations are associated with the fact that the exclusion of salts in freezing of groundwater is not included. The process of freeze-out of salts is, however, included in the 2D modelling (Hartikainen et al. 2010, Brandefelt et al. 2013).

The main permafrost modelling study performed for SR-PSU is the 2D study presented in Brandefelt et al. (2013). This study used pessimistic assumptions regarding surface and climate conditions (i.e. the assumption of dry climate- and surface conditions), as analysed and obtained from SR-Site (Hartikainen et al. 2010). For further detailed descriptions of the handling of uncertainties related to e.g. surface conditions, see Brandefelt et al. (2013), Hartikainen at al. (2010) and the **Data report**. Also the air temperature data, produced by climate model simulations and used as input to the permafrost model, has significant uncertainties. These are discussed and analysed in detail in Brandefelt et al. (2013). For the permafrost simulations performed for SR-Site for the last glacial cycle, the uncertainties in the air temperature curve were described discussed and analysed in detail (SKB 2010b, Appendix A, Hartikainen et al. 2010, **Data report**).

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

The uncertainty in geothermal heat flow was investigated and described in Sundberg et al. (2009). In general, the uncertainties in thermal characteristics of the bedrock and geothermal heat flow have a significantly smaller impact on modelled permafrost and freezing depths than uncertainties related to ground conditions and climate (Hartikainen et al. 2010).

2.2.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

3 Hydraulic processes

3.1 General

The first section of this chapter describes processes related to groundwater flow. The second section is concerned with the migration of gases (gas flow). Details concerning modelling approaches and the equations upon which the flow of groundwater and the migration of gases are built, are the same as for the safety assessment SR-Site (SKB 2010e). In this regard the Geosphere process report for SR-Site (SKB 2010e, Chapter 3), is a key reference also for the SR-PSU safety assessment.

Three major differences between SR-PSU and SR-Site are:

- Type of radioactive waste: short-lived low and medium-level (SR-PSU) vs. long-lived high-level (SR-Site);
- Location depth: shallow (SR-PSU, c. –50 m to –140 m elevation) vs. deep (SR-Site, c. –500 m elevation); and
- The SFR extension will be situated in rock below sea during at least 500 years, while the deep repository for spent fuel will be situated below land from the onset of its construction.

However, the last difference is only valid during the next c. 1,000 years due to the ongoing shoreline displacement (**Biosphere synthesis report**, Chapter 5).

3.1.1 Hydrogeological evolution

Groundwater flow in the Fennoscandian Shield is affected by changes in the climate. The presence of an ice sheet and its basal conditions significantly alters the groundwater flow regime. In periods of cold climate and beneath cold-based ice sheets, perennially frozen ground may develop. 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 margin (cf. Section 2.2, Figure 2-2). Together these factors will cause shoreline displacements and the boundary conditions for groundwater flow will change.

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 **Climate report**. Below, a brief summary of the expected hydrogeological impacts of different climate conditions during a glacial cycle is presented.

Temperate climate conditions

During the early phases of an interglacial, a fast fall of shorelines can be expected due to high rates of glacial rebound. During later phases of an interglacial, the increase in global sea levels will cause rising shorelines in areas where the isostatic depression is limited. In areas where the isostatic depression is large, the fall of shorelines will continue at a successively lower rate. During glacials, the shoreline of the contemporary Baltic Sea is determined by the location of the ice sheet margin and the connection to the Atlantic Ocean (see the **Climate report**). Likewise, its salinity is also determined by its connections to the ocean, such that it may exist as a freshwater lake rather than a marine or brackish sea, cf. the historic stages of the Baltic basin during Holocene time (see Table 7-3 in Aquilonius 2010, for a summary).

During periods of temperate conditions, the main factor of importance for groundwater flow is shoreline displacement. 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 previously associated with discharge can be transformed to recharge areas. 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 water table to follow the topography.

Periglacial climate conditions

During periods of permafrost, the main factor of importance for groundwater flow is the extent of perennial frozen ground. As the water freezes in the formation of perennial frozen ground, exclusion of salt occurs could give rise to a zone of increased salinity beneath the advancing freezing front (see Sections 2.2 and 5.11).

Frozen ground can be regarded more or less as impermeable, and the presence of permafrost and a seasonally frozen active layer restricts the infiltration of meteoric water and its recharge to groundwater systems. 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.

Glacial climate conditions

During periods of glacial climate conditions, groundwater flow will be governed by the ice sheet and subglacial layer hydrology. The conditions for groundwater flow will be determined by the configuration of the subglacial hydrological system of the ice sheet, which can be either a fast or slow flow system, or both. 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.

The presence of an ice sheet will also alter the near-surface rock stresses and, especially under a warm-based ice sheet, high water pressures can be expected. The altered effective stress state will affect near-surface fractures and fracture apertures. Fractures may grow and it is even possible that new fractures may form (see Chapter 4). Thus, the conductive features of the near-surface bedrock realm 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 spatial distribution of the deposits, but the properties of each category of deposit are expected to remain within their current ranges.

3.2 Groundwater flow

3.2.1 Overview/general description

Groundwater

Groundwater is found in voids in soils and rocks beneath the ground surface[2] regardless whether this is situated above sea level (terrestrial) or below sea level (aquatic), e.g. sea (marine). Below water and at depth below land, the voids generally contain only water – the subsurface is said to be saturated. Near the ground surface below land, there is generally a region where some of the voids contain air – the subsurface is said to be unsaturated. In the unsaturated region, the fraction of void containing groundwater generally increases with increasing depth. However, there may also be isolated saturated regions of so-called perched water within the unsaturated region. These result from spatial variations in the soil properties. Figure 3-1 shows a simplified schematic of the hydrologic cycle and the occurrence of subsurface and surface water.

The water table is the level at which the pressure in the groundwater is atmospheric. In the absence of perched water, the water table 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 and comes to the surface at marshes, streams, rivers, lake margins and sea-coasts (see below).

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

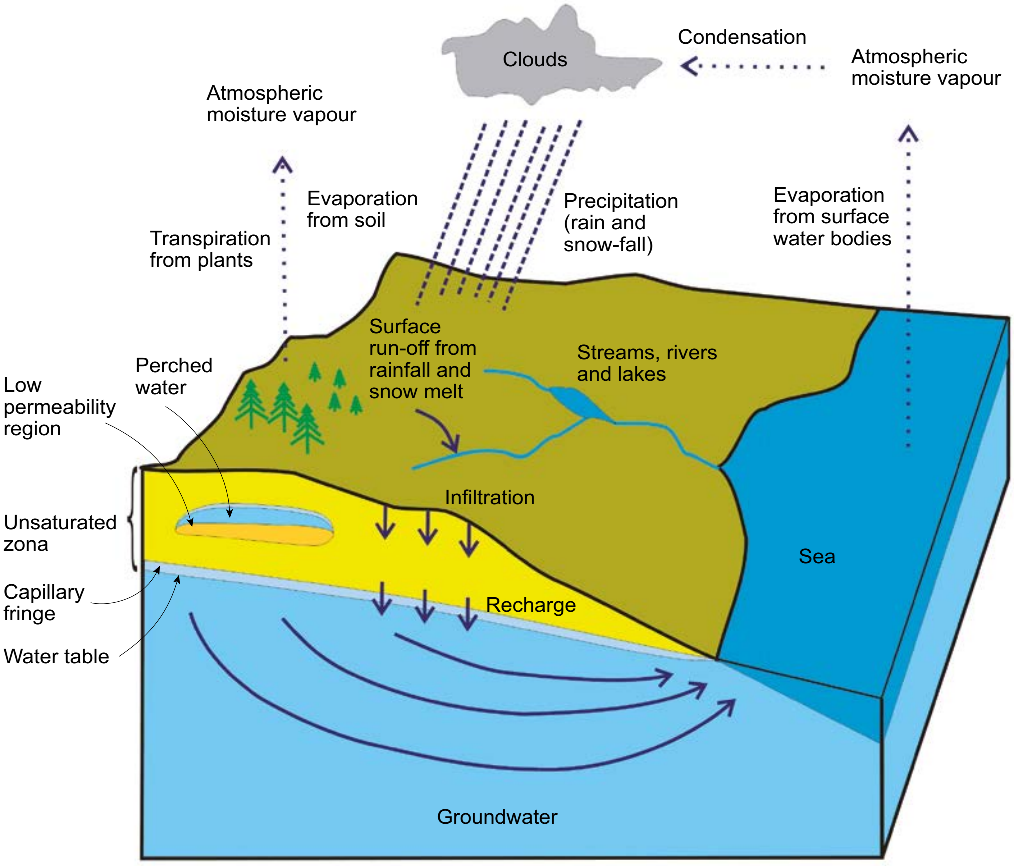

__Figure 3-1.__ Simplified schematic of the hydrologic cycle and the occurrence of subsurface and surface water. NOTE: A new version of this figure, including discharge on land, will be included.

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

The hydraulics of groundwater is described in many standard textbooks such as Bear (1972), Freeze and Cherry (1979), de Marsily (1986) and Domenico and Schwartz (1998). The SR-Site Geosphere process report (SKB 2010e, Section 3.2) gives a comprehensive description of the hydraulic processes, including mathematical descriptions and information on different modelling approaches on groundwater flow.

Following this general section, interactions with groundwater flow and geosphere variables are summarised in Table 3-1 and Table 3-2.

The hydrologic cycle

The hydrologic cycle is shown as a simplified flow net in Figure 3-2. In summary:

Water evaporates from seas, lakes, rivers, streams, marshes, soils, and surfaces of vegetation, and is given off by plants (transpiration) to form water vapour in the atmosphere.

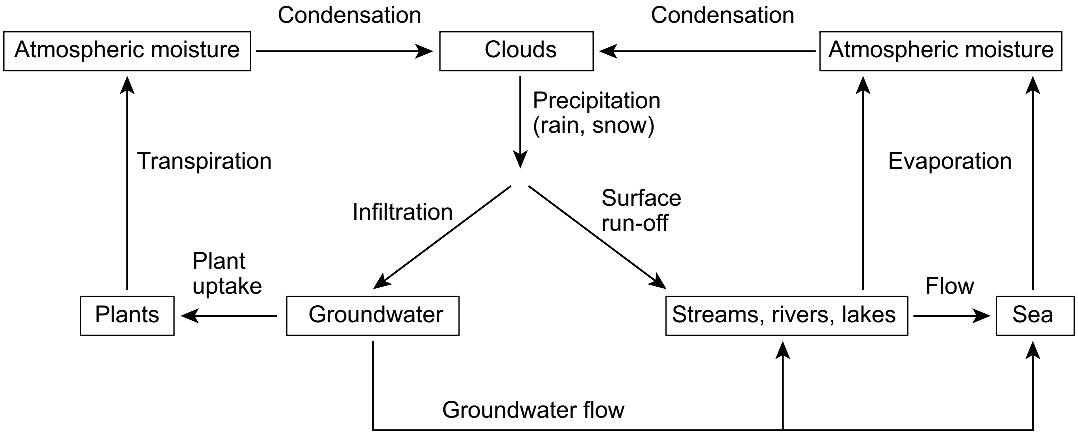

Figure 3-2. *The hydrologic cycle in a simplified form.*

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.

Beneath the water table, groundwater flows through the ground, ultimately discharging where the water table comes to or above ground surface or the sea/lake bed (Figure 3-2). This will generally be at lows in the topography. 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 proportional to the gradient of the sum of pressure and gravitational potential, and to the ability of the rocks to transmit groundwater – that is, how permeable the rocks are. Further it is inversely proportional to the groundwater viscosity. The gravitational force is proportional to the groundwater density. The empirical finding that describes the relationship between these quantities is called Darcy's law and may be written as:

$$q_x = -\frac{k_{xx}}{\mu}\frac{\partial p}{\partial x}$$

$$q_y = -\frac{k_{yy}}{\mu}\frac{\partial p}{\partial y}$$

$$q_z = -\frac{k_{zz}}{\mu}\left(\rho g + \frac{\partial p}{\partial z}\right)$$

where q (m/s) is the specific discharge (flow rate across a unit area), p is the fluid pressure (kg/m/s^2), g (m/s^2) is the gravitation, ρ (kg/m^3) is the fluid density, μ (kg/m/s) is the fluid viscosity, and k (m^2) is the rock permeability.

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 crystalline bedrock and the Quaternary deposits (glacial till mainly) is often low. Consequently, groundwater tends to build up to elevations where it can be discharged as runoff within the surface hydrological systems (cf. Figure 3-2).

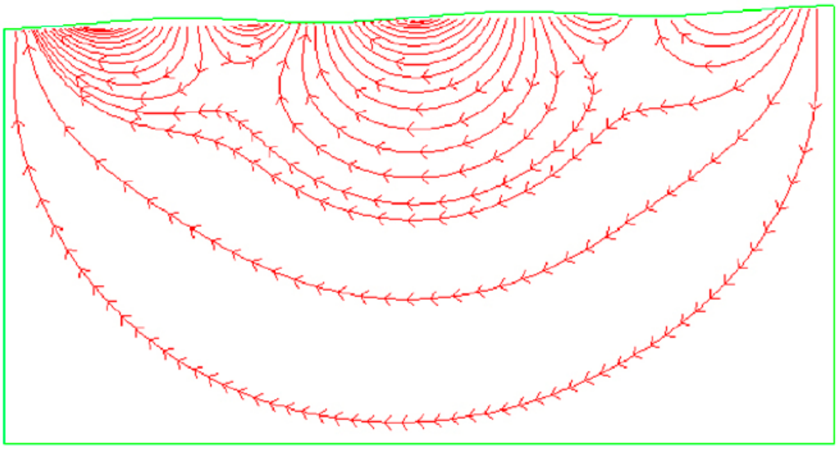

***Figure 3-3.** Example visualisation of stationary flow paths along a regional slope (topographic gradient 1/50).The length and depth of the basin is 1.2 km and 600 m, respectively. The amplitude of the undulating groundwater table is 5 m (after Werner et al. 2007).*

Furthermore, groundwater flow below land consists of local flow cells superimposed on the overall regional flow, where the near-surface flows correspond to the local flows; the flow at depth corresponds to the regional flow system (cf. Figure 3-3). Below sea, the natural hydraulic gradient is very small and flow is close to stagnant or directed upwards.

Influence of structures in the bedrock on groundwater flow

The simple pattern of groundwater flow linked to topography shown in Figure 3-3 may be modified by the presence of large-scale structures, such as deformation zones or faults. These may act as either flow conduits or barriers to flow, and result in flow cells with length scales controlled by the geometry of the structural features rather than topography (Werner et al. 2007).

Influence of salinity on groundwater flow

Typically, the groundwater salinity increases with depth, with a region of nearly fresh water near the ground surface, and brine-type conditions at great depth. The salinity is also higher beneath the sea since there is no recharge of fresh water from above except where there are islands.

The groundwater density and viscosity both increase with increasing salinity. If dense and less dense waters are present at the same elevation, the denser water will tend to flow downwards beneath the less dense water and vice versa. Thus, fresh and saline waters below land will tend to form an interface and where fresh water discharges near the coast it will flow upwards when it meets saline water beneath the sea (Figure 3-1). Where waters of different salinity fare forced to pass one another, they will tend to mix (see also Section 5.1) because of hydrodynamic dispersion and diffusion. The mixing tends to reduce the density difference and hence reduce the gravitational driving force on the flow when everything else remains the same.

Influence of temperature on groundwater flow

The bedrock temperature increases with depth because of the geothermal gradient and affects the groundwater temperature mainly through conduction. In the more permeable near-surface rock the groundwater temperature is also affected by seasonal changes in the air temperature through flow of water (advection).

The geothermal gradient is usually fairly constant (because the thermal conductivity of the rocks does not vary greatly) and is about 10°C per kilometre in Sweden (see SKB 2008a, Figure 4-9). Anomalies in the geothermal gradient can lead to local convection driven flow cells depending on the contrast (see further Section 2.1).

The increased bedrock temperature at depth will tend to counter the effect the increased salinity at depth has on the groundwater density and viscosity.

Influence of dissolved natural gases on groundwater flow

Groundwater generally contains varying quantities of naturally dissolved gas (Pedersen 2001). At the Forsmark site, nitrogen followed by helium are present in the greatest amounts, with nitrogen and carbon dioxide being most common in the more shallow groundwaters and helium in the deeper parts of the system (SKB 2008d, 2009). The concentrations of dissolved natural gases are generally low and are not considered to influence groundwater flow or the transport of radionuclides in groundwater. That is, only a separate gas phase could influence the groundwater flow.

Influence of effective rock stresses on groundwater flow

Effective rock stresses can affect groundwater flow depending on the structural–mechanical properties of the fractures, e.g. fracture orientation, fracture connectivity and fracture stiffness. If the fracture stiffness is low, an increased effective stress could decrease the fracture apertures and the fracture connectivity, hence reduce groundwater flow.

Influence of construction and operation and subsequent presence of a repository on groundwater flow

Groundwater flow is affected by the construction, operation, and subsequent presence of a repository. For instance, if the groundwater level is reduced, dissolved gases may come out of solution, e.g. as groundwater flows towards an open repository tunnel where the groundwater level would be considerably lower than the normal groundwater level at that depth due to pumping. This would lead to a region of two-phase (gas–water) flow. In this region, the rock would effectively become less permeable to groundwater, which would affect the groundwater flow during the excavation, operation and saturation periods. In addition, air may enter the rock pores and fractures immediately adjacent to the repository during excavation and operation. Furthermore, close to an open repository tunnel, the effective normal stress increases due to the reduced groundwater level, which may alter the fracture apertures depending on the fracture normal stiffness.

The repository will also be a potential source of gas (see the **Waste process report**). The generated 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 is produced, in which case it would have negligible impact on the groundwater flow (see Section 3.3).

Influence of human actions on groundwater flow

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. Vaults, tunnels and shafts are likely to have a similar, but larger effect on groundwater flow than water abstraction from boreholes. Activities that may impact groundwater flow are further discussed in the **FHA report**.

3.2.2 Dependencies between groundwater flow and geosphere variables

In this section, dependences between groundwater flow and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. Furthermore, it is indicated during what time period, climate domain, or event that the described influence is valid.

Table 3-1 outlines if/how groundwater flow is influenced by the defined geosphere variables whereas Table 3-2 outlines if/how the groundwater flow influences the defined geosphere variables.

In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. The nature of the influence between the process and each geosphere variable is elaborated upon below.

It is noted that the hydrogeological modelling conducted within SR-PSU excludes the excavation, operational, and saturation periods, since these time periods imply flow to the repository rather than from the repository. In addition, the resaturation of SFR will be so rapid since the facility is submerged, that details of the saturation process can be neglected in the evaluation of repository safety.

Table 3-1. Influences of defined geosphere variables on the process "groundwater flow" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in 3.2.7)
Temperature in bedrock	Yes.	All	The effect on groundwater density and viscosity is neglected. Freezing of groundwater is considered in the SR-PSU hydrogeological modelling.
Groundwater flow	–	–	–
Groundwater pressure	Yes.	All	The effect of pressure gradients on flow is included in the SR-PSU hydrogeological modelling.
Gas phase flow	Yes.	E/O/S	The saturation sequence is not modelled in SR-PSU.
		T/P/G	Gas flow is neglected in the SR-PSU hydrogeological modelling.
Repository geometry	Yes.	T/P/G	A detailed representation of the repository layout and its properties are included in the regional flow model. An even more detailed representation of the waste packages is included in the near-field flow model.
Fracture and pore geometry	Yes.	T/P/G	Site-specific descriptions of the fracture zone geometry and fracture network are included in the SR-PSU hydrogeology models. The fracture geometries are assumed to be constant in each realisation throughout repository evolution, but fracture geometry varies between realisations of the rock.
		EQ	Groundwater flow in response to earthquakes (that may evoke changes in fracture geometry) is not modelled.
Rock stresses	No, but indirectly through: Fracture and pore geometry.	All	–
Matrix minerals	No.	All	–
Fracture minerals	No, but indirectly through: Fracture and pore geometry.	All	–
Groundwater composition	Yes.	All	Effects of groundwater salinity on groundwater flow are neglected in SR-PSU hydrogeological modelling (Odén et al. 2014).
Gas composition	No.	All	–
Structural and stray materials	Yes.	All	The resistance due to grouting is not accounted for in the flow modelling.
Saturation	Yes.	E/O/S	The saturation of tunnels after closure is not modelled in SR-PSU.
		T/P/G	Fully saturated conditions are assumed in the bedrock, although part of the water may be frozen near the surface. When the ground surface is above the sea level, the near-surface unsaturated zone is considered in surface hydrology modelling, as it could influence maximum potential recharge (precipitation less evapotranspiration).

Table 3-2. Direct influences of groundwater flow on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 3.2.7)
Temperature in bedrock	Yes.	E/O/S T/EQ	Neglected, as the effect is small.
		P/G	Considered when assessing the distribution of perennially frozen ground.
Groundwater flow	–	–	–
Groundwater pressure	Yes.	All	The groundwater pressure is calculated using groundwater flow models.
Gas phase flow	Yes.	All	Gas phase flow is not modelled in SR-PSU. Gas residence time is set to zero.
Repository geometry	No.	All	–
Fracture and pore geometry	No, but indirectly through: Groundwater composition and groundwater pressure.	All	–
Rock stresses	No, but indirectly through: Groundwater pressure.	All	Neglected, because the effect is generally small.
Matrix minerals	No, but indirectly through: Groundwater composition.	All	–
Fracture minerals	No, but indirectly through: Groundwater composition.	All	–
Groundwater composition	Yes.	All	Output from hydrogeological modelling (flow path length, residence time, etc.) is used as input in hydrogeochemical modelling (Román-Ross et al. 2014).
Gas composition	No, but indirectly through: Groundwater composition.	All	–
Structural and stray materials	No, but indirectly through: Groundwater composition.	All	–
Saturation	Yes.	E/O	The degree of saturation is not modelled during the repository saturation process.
		T/P/G	Fully saturated conditions are assumed at depth. When the ground surface is above the sea level, but is unfrozen and not covered by an ice sheet, the near-surface unsaturated zone is included in surface hydrology modelling.

Explanation of Table 3-1

Temperature in bedrock

The influence of bedrock temperature is described in Section 3.2.1. The effect on groundwater density and viscosity is neglected in the hydrogeological modelling. Freezing of groundwater is considered in the SR-PSU permafrost simulations.

Groundwater flow

The process is the same as the geosphere variable.

Groundwater pressure

Gradients in groundwater pressure provide one the forces driving groundwater flow. The other being gravitation, see Section 3.2.1.

Gas phase flow

As described in Section 3.3 the effect of the relatively small gas flows expected in the SFR host rock at saturated conditions can be neglected. During repository saturation, there may initially be an unsaturated zone around the repository that could influence the groundwater inflow. However, the saturation of SFR is so fast since the facility is submerged that details of the saturation process can be neglected in the evaluation of repository safety.

Repository geometry

The repository geometry affects the flow because the backfilled tunnels and surrounding EDZ may provide permeable paths through the rocks and additional connections between the fractures.

Fracture and pore geometry

The fracture zones and fracture network provide the geometrical framework for the modelling of groundwater flow both on a small scale and a large scale. In the former case, geometric properties such as fracture aperture, as well as fracture network tortuosity and connectivity are of importance. In the latter case, the geometries (strike and dip) and the intersections of large fracture zones and hydraulic thickness are of importance. Different realisations of the rock are performed as means to represent parameter uncertainty due to fracture heterogeneity of the rock domain.

Effective rock stress

The effective rock stress may affect the fracture geometry (e.g. the aperture), and in an indirect manner the groundwater flow (SKB 2013b). This is thought to have an insignificant impact for a fully saturated repository compared to other processes during periods of the temperate and periglacial climate domains (Martin and Follin 2011). Changes in groundwater flow in response to open repository conditions, to glacial climate conditions or to earthquakes (which are coupled to rock stresses) are not modelled in SR-PSU.

Matrix minerals

The minerals of the rock matrix are not expected to affect groundwater flow.

Fracture minerals

The local fracture geometry may be affected by precipitation and dissolution of fracture minerals. In a natural system, such changes are slow and can be neglected. For the SFR host rock, the question has been raised whether interactions between groundwater and cementitious materials (emanating from SFR), have the potential to give rise to an alkaline high pH plume, that may cause precipitation on the safety assessment time scale (see Sections 5.6 and 5.8).

Groundwater composition

The chemical composition, primarily salinity, affects groundwater density and viscosity. Uneven distribution in salinity may give rise to density driven flow, and in case of very saline water (brine) at depth the increased salinity may to a very minor extent decrease groundwater flow (this is partly counteracted by the higher temperature at depth). However, highly saline waters such as brines are not present in the bedrock surrounding the relatively shallow SFR repository which is situated between –60 and –140 m elevation.

Gas composition

The gas composition does not affect groundwater flow.

Structural and stray materials

Grouting will reduce the groundwater flow between the host rock and repository. However, as the impact of grouting is only deemed important for the operational phase, its effect is neglected in SR-PSU.

Saturation

During the saturation period after closure, the changing degree of saturation affects the flow in the host rock near the repository. The inhomogeneous saturation affects the effective permeability and hence the flow. After the saturation period, the fracture system and the repository are assumed to be fully saturated. During cold climate periods (e.g. periglacial and glacial climate domains), part of the water may be frozen, which impacts the groundwater flow.

Explanation of Table 3-2

Temperature in bedrock

In principle, heat is transported by flowing groundwater, as well as by conduction through the rock mass. Generally, conduction through the rock mass is the most prominent heat transport mechanism in sparsely fractured rock. However, locally around flow paths the heat transported by flowing water may affect the temperature. This is of importance when assessing the distribution of perennially frozen ground.

Groundwater flow

The process is the same as the geosphere variable.

Groundwater pressure

Groundwater flow does not affect groundwater pressure; however, there is a mutual dependency between flow and pressure. That is, if you e.g. abstract or inject water into an aquifer, the pressure will be affected.

Gas phase flow

In principle, gas phase flow is driven by buoyancy forces and a physical description of this flow requires a consideration of relative permeabilities. However, gas phase flow during repository saturation is so fast that details need not to be considered when assessing repository safety. Gas phase flow resulting from gas produced in the repository is so fast compared to the groundwater flow that its residence time pessimistically can be set to zero (see Section 3.3).

Repository geometry

Groundwater flow does not affect the repository geometry.

Fracture and pore geometry

Groundwater contains solutes and groundwater flow may, through groundwater chemical composition, affect the precipitation and dissolution of fracture minerals, (cf. Section 5.6), particularly in the proximity of unsaturated engineered constructions.

The effect of high fluid pressures beneath an ice sheet that may cause hydraulic jacking of fractures, and affect the fracture aperture, is not relevant for SR-PSU because glacial climate conditions are not modelled for reasons stated in the hydrogeological modelling report (Odén et al. 2014). The effect of hydraulic jacking is further discussed in SKB (2010e, Chapter 4).

Effective rock stress

Groundwater flow affects rock stresses indirectly through the contribution of the groundwater pressure to the effective stress. For example, increases in pore pressure may generate effective stress reductions that possibly could lead to slip on critically oriented fractures. For pore pressure variations associated with saturation and desaturation of the repository host rock, the impact of that slip on stresses would be local and modest. In summary, the expected changes in groundwater pressure during temperate and periglacial climate conditions are generally so small that they have a negligible effect on the rock stresses. (The stress changes are greater in the rock during repository desaturation and saturation and during glacial climate conditions.)

Matrix minerals

The groundwater will carry solutes and may, through groundwater chemical composition, affect the dissolution (and precipitation) of matrix minerals. This process is thought to be very slow in natural systems (see Section 5.3).

Fracture minerals

There will be phases that will dissolve and precipitate as groundwaters with different composition move around, i.e. iron(III), oxihydroxides and calcite (cf. Sections 5.2 and 5.6). The characteristic reaction time of their precipitation/dissolution reactions is quite short compared to the residence time of groundwaters.

Groundwater composition

Groundwater composition is affected by the dissolution/precipitation of fracture minerals. Hence, groundwater flowing from different parts of the geosphere will have different compositions based on past water/rock interactions and present fracture/water interactions (cf. Sections 5.2 and 5.6).

Gas composition

Dissolved gases transported by flowing groundwater may come out of solution where the pressure falls.

Structural and stray materials

Structural and stray materials (e.g. grouting, rock bolts) are primarily thought to lose their function through chemical erosion, and not as result of mechanical erosion due to an increased water flow.

Saturation

Groundwater flow into or out from an unsaturated zone may affect the degree of saturation. For the SFR repository at depth, this is only of importance for the short saturation period upon repository closure. For the surface hydrology, the degree of saturation may change as response to the flow situation (which in turn is affected by shore level displacement, changing regolith geometries, evapotranspiration, etc).

3.2.3 Boundary conditions and time perspective in SR-PSU

Figure 3-4 shows the boundary conditions suggested for groundwater flow modelling during temperate climate conditions in SR-PSU. The key boundary condition is that on the top surface. Due to the shoreline displacement the terrestrial area grows rapidly in the base case scenario.

It should be noted that groundwater flow during temperate climate conditions considers timescales of many thousands of years which implies that the key hydrological process is the shoreline displacement. Day-to-day and seasonal fluctuations are of lesser interest. It should also be noted that recharging groundwater is fresh over the land surface which implies a substantial flushing of the geosphere. Since the repository depth considered in SR-PSU is shallow and since the groundwater in uppermost bedrock where the repository is situated is of very low salinity, it is a reasonable approximation to assume a uniform groundwater density at all times (cf. Stigsson et al. 1999, Holmen and Stigsson 2001, SKBdoc 1395349).

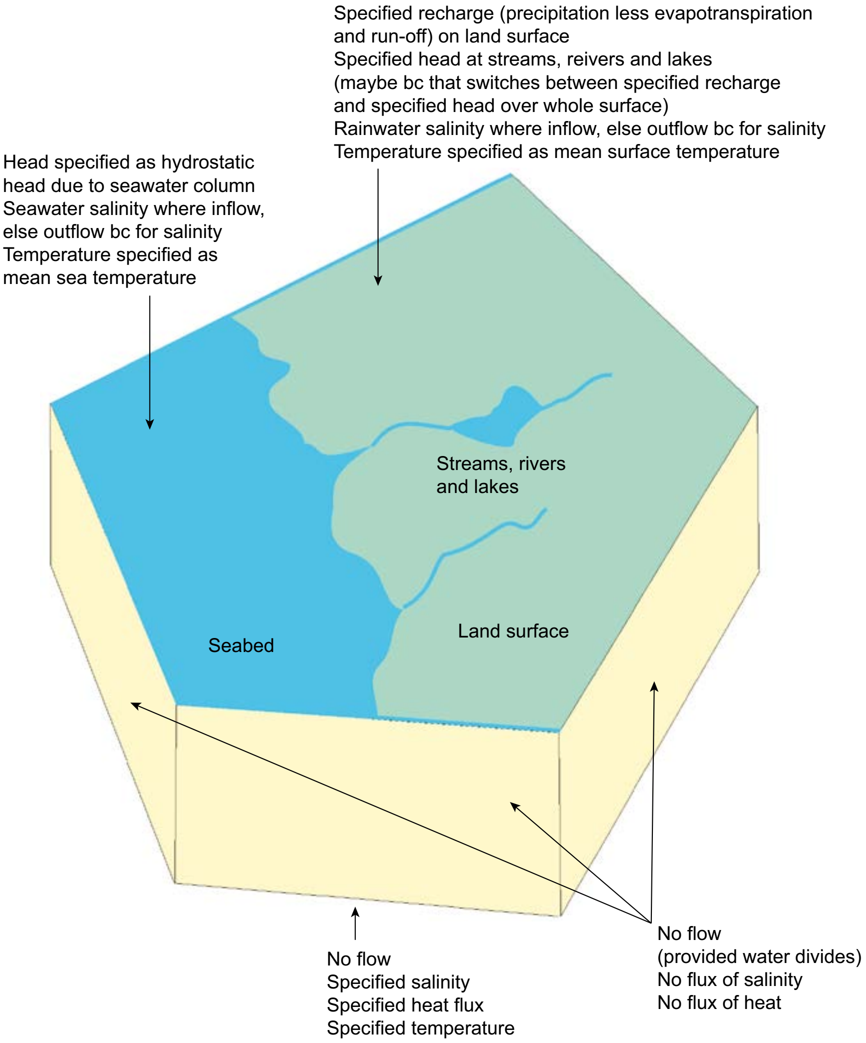

Figure 3-4. *Boundary conditions for a regional model.*

In SR-PSU, it is assumed in the groundwater flow modelling for the bedrock during temperate climate conditions that the groundwater levels at onshore discharge locations (springs, marshes, streams, rivers, and lakes) equal the surface water levels. Offshore, it is assumed in SR-PSU that the groundwater level is zero, i.e. that pressure at a submerged location corresponds to the hydrostatic pressure of the column of sea water at that location.

In Sweden, the water table is generally close to the ground surface and the unsaturated zone is thin. Measurements of groundwater levels in the candidate area for the spent nuclear fuel repository in Forsmark are within about 1 m of ground surface in the Quaternary deposits (Johansson 2008). It is assumed in SR-PSU that this situation will also apply to the present-day submerged parts of the model area once these become land as a result of the shoreline displacement.

The prevailing temperate climate conditions in the Forsmark area are expected to change in the future. Different climate cases are discussed in the **Climate report** and comprise both warmer and colder climate conditions. A warmer climate implies sea level rise and a colder climate imply the opposite. Inaddition, during periglacial and glacial periods, recharge may be prevented because of the formation of permafrost. Long periods of permafrost without an ice sheet could lead to frozen conditions at repository depth. An ice sheet will stop the formation of permafrost since it insulates the ground from the cold air. The appropriate physical boundary condition beneath a thick ice sheet may be a groundwater pressure corresponding to the weight exerted by the ice sheet, or a specified recharge (allowing for loss to subglacial streams). Information about conditions beneath an ice sheet may be provided by ice-sheet models, see Vidstrand et al. (2010a) for a literature overview and model simulations.

3.2.4 Model studies for groundwater flow

In SR-PSU, the groundwater flow modelling during periglacial climate conditions assume a specified value of the heat flux from depth. At the top of the model, the boundary condition is a prescribed value of the temperature corresponding to mean annual ground surface temperature. This approach is simplified and ignores thermal effects caused by e.g. variations in air temperature, snow cover, vegetation, soil moisture etc. However as shown in Vidstrand et al. (2010a), assessed this approach in the groundwater modelling produce results of permafrost thichness within the bounds for accessed climatic and meteorological uncertainties in Hartikainen et al. (2010). The balance between the geothermal heat flux and the permafrost process is by and large a one-dimensional process. Hence, an appropriate boundary condition on the lateral boundaries of the regional model is; no flux of heat through the vertical (lateral) boundaries. Furthermore, the permafrost development is simulated by altering the hydraulic conductivity of the subsurface with regard to simulated temperature distribution in the Quaternary deposits and the bedrock (Vidstrand et al. 2013, 2014).

Finally, the groundwater modelling in SR-PSU does not consider the excavation, operation or re-saturation periods, hence, the impact of an open repository on the groundwater flow system is not addressed in this text.

3.2.5 Natural analogues/observations in nature

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

To explore the geological, geophysical, hydrological, hydrochemical, and structural effects anticipated from the use of a large crystalline rock mass as a geologic repository for nuclear waste, the Stripa Mine Project, an international field investigation and modelling project of the conditions at the Stripa Mine, was initiated collaboratively in 1980 by Canada, Finland, France, Japan, Spain, Sweden, Switzerland, the United Kingdom, and the United States. Part of the investigations at Stripa aimed at determining the evolution of the groundwater and to establish a general programme for water sampling and analysis in crystalline rock. Water samples were taken from a maximum depth of 1 200 metres below the surface. One primary conclusion reached in these Studies so far is that different dissolved constituents will provide different residence times. This is because they have different origins and different evolutionary histories that may or may not be related to the overall evolution of the groundwater itself. Age determinations of groundwater should therefore be interpreted with this in mind.

To advance the understanding of hydrological and hydrochemical processes associated with glaciation and their impact on the long-term safety of geological repositories, the Greenland Analogue Project (GAP), a four-year field and modelling study of the Greenland ice sheet and geosphere conditions, was initiated collaboratively by SKB, Posiva and NWMO in 2010. In this study, detailed observations of permafrost characteristics are made, as well as studies of the coupling to bedrock thermal characteristics and hydrogeological and hydrogeochemical conditions (Harper et al. 2011), see Section 2.2.5 for more details.

Palaeohydrological simulations have become an important tool (SKB 2004, 2005, 2008d, Vidstrand 2010a). 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.

3.2.6 Time perspective relative to SR-PSU

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 and melting. In SR-Site, however, only the average flow system over periods of years or longer is addressed. As stated previously the groundwater modelling in SR-PSU does not consider the excavation, operation or re-saturation periods, hence, the impact of an open repository on the groundwater flow system is not addressed in this text.

During the assessment period of a hundred thousand years, the flow system will change as a result of altered climate-related conditions. Climate changes continuously and the climate conditions in Sweden can be expected to change between temperate-, periglacial- and glacial climate domains during the assessment period (**Climate report**). The inferred perturbation of natural climate change by the emission of greenhouse gases may, together with known future orbital parameters, result in an exceptionally long initial temperate period in Fennoscandia and elsewhere.

The discharge position locations may change over time if climate changes. This would be mainly as a result of the combined effects of the changing surface elevation and changing sea level, leading to changes to the shoreline and the development and/or loss of lakes and rivers. Changes to the Quaternary deposits might also affect the positions of discharge locations. These processes are included in the groundwater flow modelling for SR-PSU.

3.2.7 Handling of groundwater flow in the safety assessment SR-PSU

Below, the description of the handling of groundwater flow in SR-PSU is divided into three parts. First, the chosen modelling approach is described. Second, issues concerning different time periods, climate domains, and events are addressed. Third, issues concerning each of the geosphere variables in Table 3-1 and Table 3-2 are elaborated upon.

Handling of fractured rock as a porous medium

Groundwater flow in SR-PSU is modelled as flow through an equivalent porous medium (ECPM). The hydraulic properties of the computational grid of the ECPM model are based on up-scaling of the structural–hydraulic properties of the discrete fracture networks (DFN) and deformation zones assessed in SDM-PSU (SKB 2013b).

Handling relative to time periods, climate domains, and events

Excavation/operation/saturation period

This period includes the excavation and operation of the repository and the period after repository backfilling and closure, when the repository saturates. 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 SR-PSU, no modelling of salinity is performed by using hydrogeological models. Accordingly, no modelling of the groundwater flow at excavation and operation is required. The saturation sequence of the SFR rock vaults is assumed to be so quick, on a safety assessment time scale, that the repository is assumed to be immediately saturated upon closure. Accordingly, no hydrogeological modelling of the saturation period is performed.

Temperate climate conditions

The flow model takes account of the change in the position of the shoreline over time and the associated evolving landscape. In effect, the flow simulations are carried out, until the flow system has developed into a steady-state-like situation, which occurs at about 9000 AD (Holmén and Stigsson 2001, Odén et al. 2014).

The main inputs to the flow calculations are the site-descriptive models of the SFR site (SKB 2013b) and the candidate area for the spent nuclear fuel repository in Forsmark (SKB 2008d), landscape model (Strömgren and Brydsten 2013) and the tunnel layouts.

Periglacial climate conditions

In the SR-PSU assessment, calculations are carried out to assess the groundwater flow pattern during a period when there is permafrost in the near-surface rocks, which will act as a barrier to groundwater flow. The main input to the simulations is the site-descriptive models (SKB 2013b).

Glacial climate conditions

The periods with Glacial climate conditions are not a part of the SR-PSU assessment as the SFR-repository during these periods either will be frozen or have discharge areas to the "Baltic Sea" for reasons state in the hydrogeological modelling report (Odén et al. 2014).

Earthquakes

The effect of earthquakes on the groundwater flow is not modelled in SR-PSU. Instead pessimistic assumptions are used in subsequent radionuclide transport modelling. The most pessimistic assumption is that the water residence time and flow path length in the geosphere is zero. A less overly-pessimistic assumption may be that the flow path length equals the repository depth.

Handling relative to geosphere variables

Temperature in the bedrock

In principle, groundwater flow affects temperature in the bedrock because heat is transported by flowing groundwater. However, the rocks at depth in Forsmark have relatively low permeability and low porosity, and so the overall heat transported by flowing groundwater is small in comparison with that transported by conduction through the rocks (see Section 2.1). The temperature in flow paths, and in flow path adjacent rock, may be affected by the heat transported by flowing water. This affects the distribution of perennially frozen ground, which in turn greatly affects the groundwater flow at periods of cold climate. The distribution of perennially frozen ground, and its effect on groundwater flow, during periods of the periglacial climate domain is simulated using the DarcyTools code, which includes heat transport by groundwater flow (Svensson et al. 2010).

The temperature in the bedrock affects the groundwater flow through the effect of temperature on the viscosity and density of the groundwater. The viscosity and density are also affected by the groundwater salinity, but in the non-saline to brackish groundwater of the relatively shallow SFR host rock this effect can be neglected (cf. Chapter 5). The decay heat generated from the radioactive waste in SFR is insignificant (**Waste process report**). Accordingly, it is not expected to influence groundwater temperature at repository depth. Therefore, no variation in density is expected that would lead to buoyancy forces and convection cells in the vicinity of the repository. This justifies to not include density driven flow in hydrogeological modelling in SR-PSU. By using the same arguments, the groundwater is simplistically assumed to have a constant viscosity throughout repository evolution. (cf. Section 2.1).

Groundwater pressure

Gradients in groundwater pressure provide one of the forces driving groundwater flow. The groundwater pressure is therefore included in all hydrogeological modelling within SR-PSU.

Gas phase flow

If both gas and groundwater are present in the pores and fractures in the rock, the flows of gas and groundwater are coupled. At depth, the host rock is assumed to be fully saturated directly upon repository closure. The amount of gas that flows through the geosphere, as produced naturally or in the repository, are in SR-PSU assumed to be small enough not to affect groundwater flow.

Repository geometry

The repository geometry affects the flow because the backfilled tunnels may provide permeable paths through the rocks and additional connections between the fractures. The repository layout and the properties of repository system components, such as the hydraulic conductivity of the backfilling material, are included in the SR-PSU hydrogeological models.

Fracture and pore geometry

The fracture geometry is assumed to be constant throughout repository evolution in SR-PSU hydrogeological modelling. This means that the models do not incorporate possibly variation in response to 1) precipitation and dissolution of minerals, 2) increased rock stress and water pressure during glaciation, 3) reactivation and fracturing as response to, for example, earthquakes (cf. Chapter 5, e.g. Table 5-4).

Furthermore, the groundwater flow is assumed to be blocked by ice in the fracture system during periods of colder climate (see Section 2.2), but unaffected by short-lived and local gas pockets in the fracture system (see Section 3.3).

Rock stresses

Changes in rock stress are assumed not to affect the groundwater flow, as constant fracture geometry is assumed in SR-PSU.

Matrix minerals

The matrix minerals do not affect the groundwater flow.

Fracture minerals

Changes in fracture mineral geometry, as result of precipitation and dissolution, are assumed not to affect the groundwater flow, as constant fracture geometry is assumed in SR-PSU (cf. Chapter 5).

Groundwater chemical composition

The groundwater chemical composition affects the groundwater viscosity and density. However, in the non-saline to brackish groundwater of the relatively shallow repository host rock, possible changes in density and viscosity, in response to changes in groundwater composition, are small. Therefore, variation in the groundwater density and viscosity is neglected in SR-PSU hydrogeological modelling.

Gas composition

The groundwater flow is on the whole considered unaffected by the low content and composition of dissolved gases.

Structural and stray materials

Structural material that may decrease the groundwater exchange between the host rock and the repository rock vaults, such as grouting and injection, may degrade quickly on a safety assessment time scale. Therefore, their effect on the groundwater flow is pessimistically neglected in SR-PSU hydrogeological modelling, throughout repository evolution.

Saturation

The saturation sequence of the SFR rock vaults and tunnels is expected to be fast. Therefore, the repository and its surrounding host rock are assumed to be fully saturated directly upon repository closure. Hence the saturation process is not addressed in SR-PSU hydrogeological modelling.

3.2.8 Handling of uncertainties

An assessment of the confidence that can be placed in the current site descriptive hydrogeological model of the Forsmark-SFR site and remaining uncertainties are described in Gómez et al. (2011). Below, uncertainties regarding the description and modelling of groundwater flow of relevance for SR-PSU are elaborated upon.

Conceptual hydrogeological understanding

Much effort has been focussed on characterising the positions and hydraulic properties of different types of geological structures in the site investigations. Measurements in the deterministically modelled deformation zones suggest large spatial variability in their hydraulic properties, and hence uncertainty in their properties away from the boreholes. Their contribution to retention in the geosphere is considered to be limited since the flow-related transport resistance in large deformation zones is assumed to be relatively low. However, uncertainties in the hydraulics of the deformation zones may have more significance for the flow between the existing SFR and the planned extension as well as for the flow between different parts of each repository, and for the locations of discharge to the biosphere.

Spatial variability in the geometric and hydraulic properties of the fractured rock masses between deformation zones are handled by means of multiple unconditional stochastic discrete fracture network (DFN) realisations. In SR-Site (SKB 2011), the nature of the correlation between fracture transmissivity and fracture size was studied for different types of relationships bounded between the end members "no correlation" and "correlation without uncertainty". For SR-PSU, "correlation without uncertainty" was invoked as this rendered the most unfavourable transport simulation results in SR-Site.

Model simplifications

The unsaturated zone is incorporated in the modelling of surface hydrology and unsaturated zone hydrology (see the **Biosphere synthesis report**). In general, neglecting the unsaturated zone in the flow modelling of the temperate and periglacial climate periods is considered to an approximation of minor importance for SR-PSU, because the groundwater table is expected to be close to the ground surface for most of the period after repository saturation when the shoreline has retreated.

In the discrete fracture network (DFN) modelling, fractures are taken as planar rectangular features with a constant transmissivity. The flow is considered to be through channels in fractures. The flow modelling in SR-PSU using an ECPM model does not give a detailed representation of such channels. However, it is judged that the ECPM model captures the main characteristics of the fracture network flow system, such as flow occurring through an often sparse network of discrete fractures of varying size and transmissivity.

Boundary conditions are approximated in various ways. For example, the lateral boundaries of the regional model are taken to correspond to groundwater divides for all time. These approximations are judged to be of minor importance as explained above.

There is some uncertainty about the detailed variation of the hydrogeological properties within the Quaternary deposits, and about long-term changes to these. The uncertainties are mainly related to the shoreline displacement and the associated potential changes of discharge locations as a result of ecological and biological processes.

3.2.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

3.3 Gas flow/dissolution

3.3.1 Overview/general description

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

It should be noted that the presence of a gas phase could generate 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 Moreno and Neretnieks (2013). The quantities of radioactive gases that are originally present in the waste 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. In SFR, corroding metals generate sufficient amount of gases to form a free gas phase (Moreno and Neretnieks 2013).

A gas phase can form if the sum of the partial pressures of all gaseous compounds in the water exceeds the prevailing pressure (plus any capillary pressure). The composition of the gas phase will be such that the partial pressures of the component gases are in equilibrium with their groundwater concentrations. The natural concentrations of dissolved gases, for example nitrogen and helium (Hallbeck and Pedersen 2008a) are, however, so low that they are typically not sufficient to form a gas phase at the water pressure prevailing at the depths in question i.e. at about 100 m below the water table. Water with dissolved gases may release the gases to form bubbles as the water seeps upward to depths where the prevailing pressure is lower than the sum of the equilibrium pressure of the dissolved gases. Bubbles may coalesce to a free gas phase. The mechanisms that govern how gas forms, how bubbles migrate, coalesce, break up again etc., are described in Rahman et al. (2009). Detailed modelling of gas migration in fracture networks of the type of rock that hosts SFR has not been reported in the open literature.

The migration of a free gas through an otherwise water-saturated sparse fracture network will take place along channels controlled by the geometry of the connected fracture network and the spatial variability of fracture apertures. Gas-phase flow paths are often subject to instabilities, with a free gas pathway collapsing and reforming, resulting in the formation of separated bubbles, known as Hele-Shaw bubbles.

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 formation and release of radionuclides in gaseous form. See also Section 6.3.4.

It is not deemed necessary at present to undertake such model development because the approach is to assume that the gas residence time is so short that the generated gas immediately reaches the biosphere and deposits the radionuclides there.

Hydrogen gas is generated by oxygen-free corrosion of iron, aluminium, and zinc present in SFR. The generation of this gas will cause the water to become saturated with dissolved hydrogen gas and bubbles of phase will then be formed (Moreno and Neretnieks 2013).

Since gas bubbles are less dense than water, they will tend to move upward towards the biosphere. The bubbles may coalesce to form larger bubbles or a more continuous gas phase, but the principle of mainly vertical gas migration under the influence of buoyancy will apply. This gas will consist of hydrogen and other gases at their equilibrium pressures. The escaping hydrogen gas may therefore be able to carry other gases as well. There will be a stripping of the other gases and potential radioactive gases will be carried to the biosphere in the gas stream. Small bubbles, smaller than the local pore size or fracture aperture, will move upward by buoyance forces. If they encounter a pore smaller than the bubbles they get stuck. Surface tension will resist deformation of the bubble and hinder it to from squeezing through a smaller pore. Such capture of bubbles will influence the pathways for water flow. As more bubbles collect they coalesce. The gas pressure gradient increases and deforms the bubble(s) sufficiently to force them through the pores. Connected continuous gas paths can form to allow the gas to escape. These paths will occupy the larger pores where the capillary forces are smallest. Water will have access to the remaining smaller pores or fractures. The presence of gas in the porous or fractured medium thus modifies the water movement.

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 6.3.

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 Neretnieks (2013). There are sites where very high gas concentrations have been encountered, up to 1 litre of gas per litre of groundwater, and where the gas composition is completely different, with hydrogen and/or methane as the dominant components (Sherwood et al. 1993, Pitkänen et al. 2004).

At the Forsmark and Laxemar sites, nitrogen followed by helium are present in the greatest amounts, with nitrogen and carbon dioxide being most common in the more shallow groundwaters and helium in the deeper parts of the system (SKB 2008d, 2009).

Repository processes that are expected to generate gases include metal corrosion, degradation of organic material and radiolysis of water. These processes produce hydrogen, carbon dioxide, and low molecular weight organic compounds, mostly methane. At SFR corrosion of iron and aluminium is the main source of gas. Degradation of organic material such as cellulose can also contribute but radiolytic gas production is negligible. The generation of gas within the repository is discussed in the **Waste process report** and in Moreno and Neretnieks (2013), where also the production and release of radioactive gases is discussed.

During the excavation and operation phases of the repository large amounts of air are present in the repository. It may be also 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 waste, the drifts and tunnels and EDZ and neighbouring rock will be entrapped at repository closure. However, the amount of air added to the repository system by the EDZ is negligible when compared with the volume of air trapped in the unsaturated porosities of the waste, concrete, backfill, and bentonite buffer surrounding the Silo. 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 considerably reduced when the repository re-saturates and the pressure is restored to the hydrostatic value at repository depth. An increasing quantity of this gas will also dissolve in the groundwater as the pressure rises on re-saturation. The oxygen in the entrapped air will react with iron, aluminium and other oxygen consuming substances leaving mainly the nonreactive nitrogen behind. Gas transport and dissolution during the re-saturation phase in general is described in an SR-Site report (SKB 2010a) for a KBS-3 repository.

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

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, in the repository, the rock 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 SR-Site Geosphere process report (SKB 2010e). 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 moves to a lower pressure region.

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

Consequences of appearance of free gas

Chemically non-reactive gases that remain in solution in groundwater are not considered to have any particular consequences for repository performance that are specific to the fact that they can exist as a gas phase. The appearance of a free gas phase, that may either be trapped locally in 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 over-pressurisation to occur depends on the gas generation rate and the gas transport capacity of the waste and near field materials and the host rock. For SFR, the barriers likely to provide the main impediment to gas release from the repository are the concrete surrounding the waste, the concrete walls in BMA and Silo and the bentonite buffer surrounding the Silo. For the Silo, openings in the top will allow the gas to escape without damaging the structure. This is further described in the **Barrier process report**.

A migrating free gas phase may include radioactive, toxic, or flammable gases, and transport of these to the surface in the gas flow may lead to human exposure to radiation, toxic materials or to flammability hazards. The transport of volatile radioactive compounds in a free gas phase is discussed in Section 6.3. For SFR, the rate of generation of hydrogen and methane, the only flammable gases 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 radionuclides dissolved in the water. Most obviously, the presence of a body of trapped gas could provide a barrier to groundwater flow; this might be particularly the case close to the repository. Several studies have suggested that flows of gas through fracture networks might induce groundwater flows. Two mechanisms have been suggested by which this might occur; by the collapsing and reforming of gas pathways, and by the entrainment of groundwater in streams of bubbles. Also, for large gas flow rate the gas bubbles, which reduce the effective density of the gas bubble–water mixture, leads to buoyancy forces, which can induce circulation cells of the water. Also, the apparent viscosity of the groundwater may be altered. Further discussion of these mechanisms and references can be found in Rodwell et al. (1999). However, no clear demonstrations of these effects in the field, or their quantification with direct relevance to SFR, are available. It is not thought likely that the quantity of gas produced in SFR would be sufficient for these effects to be significant.

Gas migration in the form of bubbles may also affect radionuclide transport by the attachment of radioactive colloidal particles to bubble surfaces. This is discussed in Section 6.3.

Some 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. Origins, reactions and fate of gases in the geosphere are discussed in Neretnieks (2013).

Gas flow and transport of dissolved gas

Free gas generated in SFR, when its pressure has risen sufficiently high compared to the hydrostatic pressure, first has to migrate out of the different waste containers. This will expel water to allow gas paths to form. There are various paths the gas could then follow. If there are conducting fractures, intersecting the location(s) where gas forms, gas could enter the geosphere fracture network directly through these fractures. Alternatively, the gas could pass horizontally along the vaults and in the backfilled headspace of the Silo, where it could move until encountering rock fractures which it can enter. Gas could also collect in the tunnel, if there are sections of the tunnel where the roof is not intersected by fractures with seeping water or the narrowness of the fracture apertures and large capillary forces restrict gas entry. Eventually the gas will build up sufficient pressure to open a path through which gas will flow. For a description of how flow paths are developed, see Nagra (2004, Chapter 3).

Throughout the gas migration, there is the possibility that some of the migrating gas could dissolve in the surrounding groundwater. The extent to which this occurs will depend on the amount of water that the free gas may interact with and how close this groundwater is to being saturated with gas.

When the gas pressure exceeds the sum of the hydraulic and capillary pressures, bubbles form. They coalesce and form increasingly larger bubbles. As long as the gas cannot escape, the bubble pressure and volume grow by expelling water from the repository constructions and fractures in the rock. At gas production rates larger than what the expulsion of water allows for; two things may happen; either the structure breaks and/or existing fractures open, or the pressure overcomes the capillary pressure in the largest fractures or pores in contact with the gas creating new voids for the gas to enter. This is accompanied by forcing the water to move out through the fracture or pore network. The rate of water expulsion is governed by transmissivity of the fractures to water flow and by conductivity of the entire connected network of fractures. If this is not sufficient to stabilise the pressure, the capillary pressure in more fractures will be overcome until a steady-state flow and pressure is reached.

The capillary pressure in a slit formed fracture can be calculated by the Young–Laplace equation. p_c is he capillary pressure (Pa or N/m^2), σ the surface tension of water (0.072 N/m at 25°C), b (m) the half aperture of the fracture and $\theta \cong 0$ is the wetting angle of water/gas/granite or concrete:

$$p_c = \frac{\sigma}{b} cos\left(\theta\right) \qquad \text{Equation 3-1}$$

In a fracture with a half aperture of 10 micrometres the capillary pressure is 7,200 Pa. This is equivalent to a hydraulic head of 0.73 m. A ten times smaller aperture generates a 10 times larger capillary pressure. These capillary pressures are in the range of expected values in rock at the depth of SFR. It is not likely that such capillary pressures will contribute to change the apertures of the fractures in the network. For this to happen the pressure would have to increase to values approaching the minimum rock stress. This is on the order of the weight of the overlying rock, about 2.5 MPa or 25 atm for a depth of 100 m.

Based on data on the hydraulic conductivity of the rock around SFR, the gas production rate, and the repository layout, it can be estimated whether or not all gas produced can be effectively evacuated from SFR.

3.3.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 3-3 outlines how the processes are influenced by other geosphere variables, while Table 3-4 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. The nature of the influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. The handling is discussed in Section 3.3.7.

Table 3-3. Direct influences of defined geosphere variables on the process "gas flow/dissolution" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 3.3.7)
Temperature in bedrock	Yes.	E/O/S T/EQ	Considered but need not be accounted for as temperature is stable.
		P/G	Gas production has essentially ceased.
Groundwater flow	Yes.	E/O/S T/EQ	Impact is small and neglected.
		P/G	Gas production has essentially ceased.
Groundwater pressure	Yes.	All	Impact is accounted for.
Repository geometry	Yes.	All	The large contact area between repository and host rock is considered.
Fracture and pore geometry	Yes.	E/O/S T/EQ	Ranges of fracture apertures, and hydraulic conductivities, are considered.
		P/G	Gas production has essentially ceased.
Rock stresses	No, but indirectly through: Fracture geometry.	All	Impact is small and neglected.
Matrix minerals	No.	All	–
Fracture minerals	No, but indirectly through: Groundwater composition.	All	–
Groundwater composition	Yes.	E/O/S T/EQ	Impact small and neglected as long as water is reducing. Potential reaction with dissolved carbon dioxide neglected.
		P/G	Gas production has essentially ceased.
Gas composition	Yes.	All	Different gas solubilities are accounted for (Moreno and Neretnieks 2013).
Structural and stray materials	Yes.	All	Gas production from rock reinforcements etc is neglected, see justification in the text.
Saturation	Yes.	E/O/S T/EQ	Impact of water expulsion is accounted for (Moreno and Neretnieks 2013).
		P/G	Gas production has essentially ceased.

Explanation of Table 3-3

Temperature in bedrock

The temperature in the bedrock affects the gas flow through the effect of temperature on the viscosity, solubility and density of the gas.

Groundwater flow

If both gas and groundwater are present in the pores and fractures in the rock, the flows of gas and groundwater are coupled. Flowing groundwater can transport dissolved gas, which may subsequently come out of solution. See also Section 3.1.1.

Groundwater pressure

The groundwater pressure is an important factor in gas flow. Gas can only enter initially water-filled fractures (and rock matrix pores) if its pressure is greater than the groundwater pressure by an amount that is inversely proportional to the fracture aperture or pore size. It is not expected that gas would enter the matrix pores in Swedish bedrock in general, because of capillary forces. The pressure will also influence the volume of the trapped gas, its density and the equilibrium concentration in water and gas. However, this will not lead to important changes for the gas flow because essentially all generated gas will escape anyway. The partial pressure in the gas and concentration of dissolved gas will be affected. Groundwater pressure at repository depth is expected to be fairly stable during the period when free gas is produced.

Gas phase flow

As the geosphere variable equals the process, the corresponding field in Table 5-11 is left blank.

Repository geometry

The repository geometry affects the gas flow because the backfilled tunnels and surrounding EDZ may provide permeable paths through the rocks and additional connections between the fractures. However, the gas can be expected to find the best escape pathways in the tunnels, little influenced by their geometry.

Fracture and pore geometry

The geometrical configuration of fractures governs the gas flow. The fracture aperture, geometry, and connectivity are key properties that determine how permeable the rock is and so play a major role in determining the gas flow. The fracture aperture is also a key control on the capillary pressure, which determines the excess pressure above the groundwater pressure) required for gas to displace water from a fracture. This is assessed and bounded by measured values of rock hydraulic conductivity.

Rock stresses

Rock stresses may indirectly affect gas flow and dissolution, through changes in fracture geometry and transmissivity. Changes to the rock stresses would affect the properties of the fractures, in particular the aperture and hence transmissivity and capillary pressure. However, the changes to the rock stresses are expected to be small except for the changes due to repository construction and re-saturation, earthquakes (on very short scales), ice-loading (on long timescales), tectonic effects (on very long timescales) and earthquakes.

Matrix minerals

Matrix minerals are not expected to affect gas flow.

Fracture minerals

The only reactive gas expected is carbon dioxide. The fraction of gas that is carbon dioxide is expected to be small (Moreno and Neretnieks 2013) so the gas flow will be little affected if the carbon dioxide reacts. However, the carbon dioxide including radioactive carbon dioxide would dissolve as carbonate ions or precipitate under the prevailing water chemical conditions and so be withdrawn from the gas.

Groundwater composition

The groundwater composition may affect the gas flow because dissolved gases may come out of solution if the pressure falls sufficiently. This will e.g. apply to carbon dioxide for which the partial pressure is influenced by pH.

Gas composition

The gas composition affects the gas phase flow properties, but insignificantly with respect to the gas flow.

Structural and stray materials

The amount of gas produced in the repository will vastly exceed that produced from structural and stray material (i.e. rock reinforcements and grouting). Grouting of the rock can affect gas escaping from the repository. As the grout is degraded over time, the permeability of the grouted rock would increase. Grouting in the vicinity of the tunnels would reduce the permeability of the rocks locally and affect the gas flow. It is likely that grouting would be focused on transmissive features, and so the local flow would be significantly affected.

Saturation

The gas flow-paths in the surrounding host rock are considerably influenced by the degree of saturation.

Table 3-4. Influences of the process "gas flow/dissolution" on defined geosphere variables, and a short indication of how this may be handled in safety assessment. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 3.3.7)
Temperature in bedrock	Yes.	All	Neglected because of limited heat transport capacity of transported gas, compared to conduction in the bedrock.
Groundwater flow	Yes.	All	Impact is minor and is neglected in hydrogeological modelling.
Groundwater pressure	Yes.	All	Impact is small and neglected.
Repository geometry	No.	All	–
Fracture and pore geometry	Yes.	All	Impact is small and neglected.
Rock stresses	Yes.	All	Impact is small and neglected.
Matrix minerals	No, but indirectly through: Groundwater composition.	All	Possibly, dissolved carbon dioxide can dissolve carbonate minerals. Impact is small and neglected.
Fracture minerals	No, but indirectly through: Groundwater composition.	All	Possibly, dissolved carbon dioxide can dissolve carbonate minerals. Impact is small and neglected.
Groundwater composition	Yes.	E/O/S	Impact of oxidation from air neglected.
		T/P/G EQ	Carbon dioxide in gas can dissolve and change pH. Impact is small and neglected.
Gas composition	Yes.	All	Carbon dioxide in gas can dissolve, which impacts the gas composition. Impact is small and neglected.
Structural and stray materials	No.	All	–
Saturation	Yes.	E/O/S	The re-saturation sequence is not modelled.
		T/EQ	Fully saturated conditions are assumed.

Explanation of Table 3-4

Temperature in bedrock

In principle, gas flow affects temperature in the bedrock because heat is transported by the flowing gas. However, the heat capacity of gas is low and the crystalline rocks at depth in Sweden have low permeability and low porosity, and so the heat transported by flowing gas is negligible in comparison with that transported by conduction through the rocks (see Section 2.1 and Section 3.1).

Groundwater flow

If both gas and groundwater are present in the pores and fractures in the rock, the flows of gas and groundwater are coupled. The gas needs only to open a minor fraction of the fractures to allow gas escape. Most of the fractures will still form a connected network to allow water to flow. Hydraulic gradients will be affected by the presence of gas paths. The overall impact on water flow is deemed to be small.

Groundwater pressure

The groundwater pressure is mostly determined by the level of the water table above the repository but is locally influenced by the groundwater flow, which is coupled with the gas flow.

Gas phase flow

As the geosphere variable equals the process, the corresponding field in Table 5-12 is left blank.

Repository geometry

Gas flow does not affect the repository geometry.

Fracture and pore geometry

If the gas pressure rises sufficiently, this could in principle lead to opening and extension of existing fractures or even the creation of new fractures. This is very unlikely.

Rock stresses

If the rock is sufficiently impermeable to prevent gas generated in the repository from migrating away from the repository, it is possible that the gas pressure could rise sufficiently to affect the stresses in the rock (and even lead to fracturing). This is very unlikely.

Matrix minerals

In principle, gases could indirectly affect matrix minerals, through their effect on the composition of groundwater flowing through the fractures, which can affect the composition of the groundwater within the rock matrix and hence may lead to precipitation or dissolution of minerals within the matrix. However, for the gases of interest, these effects are negligible.

Fracture minerals

In principle, gas flow could indirectly affect fracture minerals, through its effect on the groundwater composition and hence on rock-water interactions. Reaction of dissolved carbon dioxide with carbonate minerals can occur.

Groundwater composition

Constituents transported in gas phase may dissolve in water. Conversely, constituents in the groundwater may degas. Accordingly, the gas flow affects the groundwater composition. During excavation, operation and re-saturation, air will contact the rock and groundwater close to the underground openings, giving an oxidising effect.

Gas composition

Gas flow through waters with different compositions can affect the gas composition because different gases have different solubilities and mass transfer rates.

Structural and stray materials

Gas flow would not affect structural and stray material (such as grout used to seal fractures). In case of corrosion of rock reinforcements, there will be an associated gas flow. However, this gas flow does not limit the rate of the corrosion.

Saturation

Gas flow rate will affect the saturation in the host rock.

3.3.3 Boundary conditions

The flow rate of repository generated gas is mainly determined by the gas production rate and the hydrostatic and gas pressures at repository depth. These are the principal factors that will determine in what form the gas will be present (dissolved or as a free gas phase). The flow pattern in the geosphere is bounded by the fracture network.

3.3.4 Model studies/experimental studies

Experiments relevant to gas migration in fractured rock that is initially saturated have been conducted both in the laboratory environment and in the field. Field studies have, for example, been conducted at the Äspö HRL (Jarsjö 1998), at Grimsel (Finsterle and Pruess 1995, Marschall and Lunati 2006), at Reskajeage (Lineham et al. 1996), and at Manitoba (Gascoyne and Wuschke 1997). Gas migration in shear zones has been studied at the Grimsel test site. These investigations are summarised in http://www.grimsel.com/gts-phase-v/gam/gam-introduction. In the summary of these investigations it is concluded that the transport processes are site specific. 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 KBS-3 repository up to the surface compared with the rate at which gas is expected to be generated in a repository for spent fuel in copper canisters. Provided, therefore, that the natural fracture system is adequately connected, it is expected to constitute a rapid transport pathway for the gas. Although this is not directly comparable to the conditions at SFR the principles are the same and the same models can be used to assess gas transport from SFR.

The modelling study by Painter and Sun (2005), shows that many issues arising during the period when the repository is open can be analysed without recourse to full two-phase flow modelling. Specifically, maximum and steady-state inflows to an open repository can be predicted without major errors as long as an unconfined aquifer (free-surface model) of groundwater flow is adopted. Hence, the modelling of the open repository period performed in SR-Site (Svensson and Follin 2010), for the KBS-3 repository, considers saturated flow beneath a free surface. An indication of timescales for the re-saturation of the repository tunnels after backfilling and closure is of interest. However, it is not thought likely that a field-scale two-phase flow calculation of gas migration from a spent fuel canister through the geosphere will be appropriate. Svensson (2010) estimates the timescales for the hydration process by assuming that the hydration process of the unsaturated parts of the backfill can be modelled as a single-phase, saturated groundwater system with different specific storage for the saturated and unsaturated parts.

In contrast to the much deeper high-level waste repositories considered above, which are not yet built, at SFR-1 the conditions during the operating phase are monitored and well known because the repository exists.

3.3.5 Natural analogues/observations in nature

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

There are many studies on helium gas transport in the subsurface (e.g. Torgerson 1989, Delos et al. 2010), as well as studies on the release and transport of radon released from uranium minerals in granite (Andrews et al. 1989). The release mechanisms are understood in principle, as are the mechanisms influencing transport. However, observed helium profiles in deep boreholes have been found to be difficult to reconcile with the models used to interpret them.

There are also numerous studies addressing the capability of the geosphere to retain gases, particularly in the field of geological storage of CO_2 but these studies deal with other rock types than granites.

3.3.6 Time perspective

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 had will have dissipated by the time that the repository has become re-saturated.

Gas transport, by bubbles and by more continuous paths, will take place in different parts of the repositories and will vary in time and space because the hydrogen production by corrosion varies in time and space. Should a free gas phase pathway form throughout the geosphere, the time for gas transport from the repository to the atmosphere would be expected to be much shorter than the time for water transport, due to the much higher upward pressure gradient (buoyancy effects) for the gas. Even, if gas were transported as bubbles the timescales would still be expected to be shorter due to a short vertical pathway under buoyancy and less retention processes. The period over which gas may be generated from corroding metals in SFR is expected to be thousands to tens of thousands of years (see the **Waste process report** and the **Barrier process report**).

3.3.7 Handling in the safety assessment

In this section, the SR-PSU team gives recommendations on how to handle the process of gas flow and dissolution. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of the interaction tables are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

During the excavation and operation period of the repository, the system is characterised by the tunnels being at atmospheric pressure. Also, the re-saturation phase of the repository is included in this period, when the backfilled tunnels and Silo go from their initial partial saturation to full saturation. The re-saturation sequence is not modelled in SR-PSU. Below a few studies supporting this decision are outlined.

In a study of the importance of two-phase flow (air-water) in the behaviour of an open repository, Painter and Sun (2005) concluded that an unsaturated region may be induced in the vicinity of the tunnels during repository pre-closure operations, and that an unsaturated zone will be formed above the repository. However, for the case considered at Forsmark for the KBS-3 repository (Svensson and Follin 2010), 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. Similar conditions are expected for SFR.

Periods of the temperate climate domain

Before full re-saturation, when the drifts still have connections by gas pathways, the generated gas can flow out. When these paths have closed gas will start to accumulate and pressure will build up until it overcomes the hydrostatic head and capillary opening pressure. Then gas starts to flow and continues to do so until the gas generation rate has dropped sufficiently to allow all gas to dissolve in the seeping water which carries it away by flow. When this water eventually reaches shallower depths, some of the dissolved gas forms bubbles, which move upward.

As the gas flow in the geosphere is fast compared to the water flow, it is in SR-PSU assumed to be infinitely fast. This means that gases that enter the geosphere, from the repository, will immediately emerge in the surface system. Also, the exit locations at the surface for the gas release should be more or less directly above the repository, and do not necessarily coincide with exit locations of groundwater flow.

During early times when the Baltic still covers the site most gas will reach the sea water and either dissolve in the large water volumes or continue as bubbles to the surface of the sea where the gas is mixed with the atmosphere.

As the sea recedes the gas will instead increasingly emerge in locations not covered by water and migrate through an unsaturated soil zone, where such exists. No loss of ^{14}C to fracture minerals is assumed to occur during the gas passage to the biosphere. There reactive gases such as methane will, at least to some extent, be oxidised by oxygen in the air and form carbon dioxide. Therefore, all volatile C-14 compounds are in SR-PSU assumed to be available for uptake by vegetation (**Biosphere synthesis report**).

Periods of the periglacial climate domain

Production of gas is assumed to have ceased at periods of the periglacial climate domain and no transport of gas is modelled.

Periods of the glacial climate domain

Production of gas is assumed to have ceased at periods of the glacial climate domain and no transport of gas is modelled.

Earthquakes

It is considered that gas flow/dissolution is not relevant to the generation of earthquakes, and earthquakes are not relevant generally to gas flow/dissolution, although earthquakes could lead to the sudden release of trapped gas as a result of induced fracturing. The handling is SR-PSU is the same as during periods of the temperate climate domain.

Handling relative to geosphere variables

Temperature in bedrock

The flow and dissolution of gases is not considered when evaluating the bedrock temperature. Furthermore, as result of the simplistic handling of gas transport, the temperature is not internalised in any transport modelling.

Groundwater flow

The coupled groundwater–gas flow may be of importance during the re-saturation of the repository host rock. However, this period is not modelled. As the rock is saturated, gas is assumed not to impact the hydrogeological evolution in the SR-PSU models.

Groundwater pressure

A gas flow may vary locally and it can impact the groundwater pressure. However, this is neglected in SR-PSU hydrogeological modelling.

Gas phase flow

The geosphere variable equals the process. Accordingly, there is no interaction to handle by definition.

Repository geometry

As result of the simplistic handling of gas transport, details in the repository geometry are not internalised in the gas flow evaluation. However, it is considered that the contact area between the repository vaults and the host rock is sufficiently large so that the gas can be efficiently evacuated.

Fracture and pore geometry

As a result of the simplistic handling of gas transport, details of the fracture and pore geometry are not internalised in the gas flow evaluation. However, it is considered that fracture apertures are sufficiently large so that the gas can be efficiently evacuated.

Rock stresses

Rock stresses are assumed to have no impact on the gas flow and dissolution in SR-PSU.

Matrix minerals

Matrix minerals are assumed to have no impact on the gas flow and dissolution in SR-PSU.

Fracture minerals

Dissolved carbon dioxide can dissolve or precipitate carbonate minerals. It is assumed that gas transport and dissolution do not affect precipitation and dissolution of fracture minerals except possibly before the repository is saturated. Impact is small and neglected.

Groundwater composition

During excavation, operation, and saturation, air will come in contact with groundwater and rock, adjacent to the underground openings. Accordingly, there will be an oxidising effect and trapped oxygen will quickly be consumed by mineral reactions in the near-field during the saturation phase. However this phase is not part of the long-term handling, hence not modelled in SR-PSU.

Upon re-saturation, the interaction between groundwater and gasses, in terms of dissolution, degassing and reaction is generally neglected in SR-PSU. The exception is for the carbonate system where effects of changed pH have been considered in modelling.

Gas composition

Changes in gas composition in the geosphere are not modelled in SR-PSU.

Structural and stray materials

The gas production from structural and stray materials (rock reinforcements and grouting) is neglected in SR-PSU, as most of the gas is produced in the repository.

Saturation

Water re-saturation of the repository host rock is not modelled in SR-PSU. Contaminating gases entering the geosphere, from the repository, during the re-saturation period are assumed to immediately emerge in the surface system.

3.3.8 Handling of uncertainties

Uncertainties in mechanistic understanding

There are uncertainties in a quantitative description of gas and two-phase flow through a geosphere in which the rock permeability is provided by a network of discrete fractures. Although it is believed that the basic physics of gas migration are well understood, the application to fractured media involves considerably difficulty if details of flowpaths are desired. This is fundamentally so 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).

However, for the purposes of assessing pressures needed to evacuate all the gas generated in SFR, bounding and conservative estimates can be made with good confidence (Braester and Thunvik 1983). It is therefore not in doubt that all the gas that can be generated in SFR readily will be able to escape without increasing the pressure by more than at most half an atmosphere. This will not damage the rock but may locally influence the location of the gas paths. Details of flow paths cannot be known but these are of no concern for the present purposes.

Model simplification uncertainties

The assessment of the capacity for gas migration through the geosphere is based on simple arguments about the likely capacity of the discrete fracture network to transport gas, in relation to the gas produced in the repository. These arguments consider estimates of a reasonable range of the hydraulic conductivities required for gas to dissipate, and thereby avoid a pressure build up. Although these simple arguments avoid much of the complexity of actual gas flow channels through rough fractures with variable orientations and interconnections, the approach is robust because the results obtained with cautious assumptions do demonstrate that there is ample capacity in the fracture network to transport all the gas generated from the repository without a significant pressure build up.

3.3.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

4 Mechanical processes

4.1 General

4.1.1 Definition of mechanical processes

In this chapter, mechanical processes in the geosphere, identified as relevant to the long-term safety of the SFR repository, are described. The process descriptions are based on the initial state of the SFR, defined as its state at closure (**Initial state report**). The large-scale mechanical evolution of the shield as well as earthquakes are described in the SR-Site Geosphere process report (SKB 2010e, Sections 4.1.2 and 4.1.3, respectively). Since both repositories are planned to be located in Forsmark, these descriptions apply also for SFR.Mechanical processes are the consequence of changing boundary conditions, such as the doming of the ground surface associated with glaciation or the rapid stress redistribution that can occur during blasting of an excavation. In other words the rock mass deforms as loads are applied or removed. Mechanical processes in the rock mass affect both the intact rock and the fractures. In this chapter three mechanical processes are considered:

- Deformation of intact rock.
- Displacements along existing fractures.
- Fracturing.

In addition to the mechanical processes noted above, open fractures may be subject to deposition and/or erosion of infilling material under certain conditions. This process is coupled to groundwater flow (described in Chapter 3). Although not a rock mass mechanical process, erosion and sedimentation in fractures is considered in this chapter. The mechanical processes are described in the following.

4.1.2 Mechanical evolution

The most significant changes of the mechanical conditions of the SFR rock mass take place during excavation of the rock caverns. The stresses redistribute around the excavations and the rock deforms slightly due to stress release. Fracturing occurs in the blasted volume and some shear and normal displacements along the fractures will also follow as a result of excavation.

However, the process interactions of importance for the long-term safety of the repository focus on the mechanical processes foreseen from the period after the closure of the repository, i.e. the initial state. The processes connected to the drill and blast operations and the excavations are therefore not included here, since they are processes occurring before the initial state and should be taken into consideration in the description of initial state (**Initial state report**). Drill and blasts are not expected to occur after the initial state.

During the excavation and operational periods the bedrock temperature will vary slightly, which will cause minor changes in stresses due to thermal expansion and shrinkage. During these periods there will also be an ongoing drainage in the rock around the facility. The drainage increases the effective stresses and this will cause some closure of fractures. During the saturation phase, after closure of SFR, the pore pressure in the fractures will be restored and the fractures will experience opening displacements to a corresponding degree.

The SFR installations and structures, such as rock reinforcement, concrete waste compartments, bentonite, backfill and plugs, will be in direct or indirect mechanical contact with the rock walls. Loads from the structures, for example from the concrete plugs due to swelling pressures from bentonite backfill, will cause mechanical processes in the intact rock and the existing fractures close to these locations.

In the reference evolution, the future climate development is given by two climate cases, the *global warming* and *early periglacial* climate cases, representing prolonged interglacial conditions at Forsmark due to the combination of an enhanced greenhouse effect and future variations in insolation during the next 50,000 years (**Climate report**, Chapter 4).

In the *global warming climate case,* Forsmark is located in a temperate climate domain for the initial 50,000 years. The period from 50,000 years to 100,000 years after present is defined to describe natural climate variability during a period of global cooling, here represented by a succession of periods of a few centuries to almost 10,000 years of periglacial and temperate climate domain. The *early periglacial climate case* is defined as a variant of the *global warming climate case,* representing the lower end of the uncertainty range associated with the amount of human and natural carbon emissions. Due to a faster temperature decrease in this climate case, a period of periglacial climate domain is defined to occur in the period of minimum summer solar insolation at high northern latitudes from 15,500 to 18,500 years after present.

During the initial period of temperate climate domain in the reference evolution, there will be an on-going degradation of the reinforcements. This degradation will to some extent alter the stress distribution locally around the reinforced rock caverns. The degradation of shotcrete and rock bolts is expected to be complete within the first 250 years after closure of the repository.

In the periods of periglacial climate domain, a lower ground temperature and permafrost conditions are expected. This temperature change and the freezing process of the groundwater will lead to mechanical processes, including deformation of intact rock, fracture opening and the formation of new fractures. The near-surface air temperature evolution and associated geosphere temperatures during periglacial periods, in the *global warming* and *early periglacial* climate cases, included in the SR-PSU reference evolution, is described in the **Climate report** (Chapter 4).

The glacial climate domain is not present in the climate cases that support the SR-PSU reference evolution. However, to span the uncertainty in the timing and duration of ice-sheet growth in the Northern Hemisphere, and for comparison with earlier safety assessments for the SFR repository, a climate case representing a repetition of conditions reconstructed for the last glacial cycle is included in SR-PSU. The *Weichselian glacial climate case* serves to illustrate the possible impact of ice-sheet growth and decay on the repository safety functions. This impact is covered by a safety assessment scenario that assumes completely degraded concrete barriers and no geosphere retention (**Climate report**, Section 1.2, and **Main report**, Chapter 7).

A glaciation would imply not only an increase of the vertical and horizontal stresses in direct response to the ice load, but also horizontal stress effects (decrease and increase) caused by crustal flexure (Lund et al. 2009). However, a previous safety assessment considering a "what-if" case including a glacial event did pessimistically assume completely degraded concrete barriers and no geosphere retention after a glaciated period (SAR-08). The result from the assessment of this case was that the repository was safe even without the geosphere retention. Hence, since the barriers will be assumed completely degraded at the time of glacial conditions, displacements in intact rock and along fractures are not considered (**Radionuclide transport report**, **Barrier process report**).

The seismic activity in the Fennoscandian shield is currently very low. However, large intraplate earthquakes cannot be ruled out in a 100,000 year perspective, as evidenced by the events in New Madrid (USA), Ungava (Canada), West Australia and elsewhere (e.g. Gangopadhyay and Talwani 2003). Extrapolating[4] the magnitude–frequency estimates of Bödvarsson et al. (2006), the probability in a 100,000 year time frame of having an earthquake of magnitude 6 or larger within 10 km of Forsmark is 15%. We emphasise however, the vast uncertainties in this estimate which is based on less than 100 years of instrumentation.

4.2 Deformation of intact rock

4.2.1 General description of deformation of intact rock

Deformation of intact rock is here defined as the deformation occurring when the loads are below those associated with fracturing. In the case of intact crystalline rocks like those common in Forsmark, linear-elastic relations valid for isotropic materials are commonly used to approximate the deformations.

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[4] Such an extrapolation implicitly assumes that the frequency–magnitude relation derived by Bödvarsson et al. (2006) for the 1000 year perspective is also valid for the 100,000 year perspective, thereby neglecting eventual migrations in time and/or space of the seismic activity.

The deformations are determined by two elastic parameters, Young's modulus and Poisson's ratio. The description of these parameters for rock types in the SFR-PSU volume is given in the Site Descriptive Model (SKB 2013b). The only aspect treated in this assessment is the elastic deformation of intact rock. Plastic deformations of intact rock such as certain variants of creep, are neglected as the impact is judged to impose insignificant effects on long term safety.

4.2.2 Dependencies between intact rock deformation and geosphere variables

In this section, dependencies between this process and defined geosphere variables are outlined. Table 4-1 lists how a change in the variables influences the process, i.e. how the change directly influences deformation of intact rock. The rightmost column indicates how this influence is handled in the safety assessment SR-PSU. Table 4-2 lists instead how a change in the process directly influences the geosphere variable. After the tables additional information is provided for each variable dependency.

Table 4-1. Direct influences of defined geosphere variables on the process "Deformation of intact rock" and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No or No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.2.7)
Temperature in bedrock	Yes.	T/P/G Mainly P	Not handled. The influence of the process on radionuclide transport is judged negligible.
Groundwater flow	No.	–	–
Groundwater pressure	No, but indirectly through rock stresses.	–	–
Gas phase flow	No.	–	–
Repository geometry	Yes.	All	The geometry of the rock caverns is included in stability analyses performed.
Fracture and pore geometry	No, but indirectly through change in rock stresses.	–	–
Rock stresses	Yes.	All	Rock stresses and their influence on the process are included in stability analyses. However, the changes in the effective rock stress due to groundwater pressure changes, have not been handled.
Matrix minerals	Yes.	All	Elastic properties, determined by mineral composition, are input to any mechanical analysis.
Fracture minerals	No, but indirectly through: Fracture stiffness and rock stresses.	–	–
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	No.	All	The reinforcement is assumed degraded in the long-term perspective and therefore it is not needed to simulate the reinforcement in safety assessment. Stresses at plugs are not handled.
Saturation	No, but indirectly through: pore pressures and structural materials.	E/O/S	–

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-1

Temperature in bedrock

Temperature changes will result in intact rock deformation which will depend on the thermal expansion coefficient and the degree of confinement.

Groundwater flow

Groundwater flow is unimportant to the mechanical behaviour of the intact rock.

Groundwater pressure

Changes in groundwater pressure, causes a change in effective fracture normal stress, which could causes shear failure on fractures and thus indirectly also cause some deformation of the intact rock around the fractures. However, the direct effects on intact rock from changes in the effective stress are expected small, since the stiffness of the intact rock is high and the likely groundwater pressures low for most scenarios.

Gas phase flow

Gas phase flow is unimportant to the mechanical behaviour of the intact rock.

Repository geometry

The shape, size and orientation of the excavated rooms will contribute to determine changes in rock stresses during all time periods. Intact rock deformation will take place in response to all such stress changes.

Fracture and pore geometry

The geometry of the fracture system contributes to determine changes in the stress field, e.g. because of stress redistribution effects close to slipping fractures. Deformation of intact rock will take place in response to all such stress changes.

Rock stresses

Changes in rock stresses cause deformation of the intact rock according to the stress-deformation laws established for the different rock types. The Young's modulus for the intact rock is in the order of 70 GPa. Major stress changes may cause fracturing (see Section 4.3).

Matrix minerals

The mineral composition contributes to determine the deformation and strength properties of the intact rock. However, the variation in composition is known and fairly limited.

Fracture minerals

Fracture minerals influence the strength of the fractures and can therefore, similar to the fracture geometry, contribute to determining rock stresses.

Groundwater composition

Groundwater composition has negligible effect on the mechanical behaviour of the intact rock.

Gas composition

Gas composition is unimportant to the mechanical behaviour of the intact rock.

Structural and stray materials

The rock reinforcement consisting of rock bolts and shotcrete will deteriorate with time. This will cause redistribution of stresses, and some deformation, in the influenced rock volume around the excavations. Similarly some minor pressure may be transferred from plugs and backfill materials, and this load may cause intact rock deformation.

Saturation

Saturation changes will give effective stress changes and impact on the fracture strength and contribute to control the scope and extent of deformation (cf. groundwater pressure). Saturation will also influence load indirectly through the effect on swelling backfill materials.

Table 4-2. Direct influences of the process "Deformation of intact rock" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.2.7).
Temperature in bedrock	No.	–	–
Groundwater flow	No, but indirectly through fracture and pore geometry.	–	–
Groundwater pressure	No.	–	–
Gas phase flow	No, but indirectly through: fracture and pore geometry.	–	–
Repository geometry	No, but indirectly through: processes "displacements along existing fractures" and "fracturing".	–	–
Fracture and pore geometry	Yes. Intact rock deformation can influence the fracture apertures and may also influence fracture propagation, thus influence the network.	All	Not handled. The influence on the fracture geometry is negligible compared to the overall uncertainty and the simplifications of fracture network in the models (cf. Section 3.2).
Rock stresses	Yes.	All	The stress-strain relationship is input to all analyses performed.
Matrix minerals	No.	–	
Fracture minerals	No.	–	–
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	Yes.	All	Not handled. Influence on safety judged negligible (see below).
Saturation	No, but indirectly through: fracture and pore geometry.	–	–

***)** E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-2

Temperature in bedrock

No mechanical process will have any influence on the rock temperature.

Groundwater flow

Aperture changes, closure and opening, will take place in response to intact rock deformation. This will have some, minor, influence on the groundwater flow.

Groundwater pressure

Aperture changes, closure and opening, taking place in response to intact rock deformation will affect the groundwater flow and, as a possible consequence, the pore pressure distribution. For fully disconnected fractures, the local liquid pressure will change in direct response to opening and closure.

Gas phase flow

Aperture changes, closure and opening, will take place in response to intact rock deformation. This will have an influence on gas phase flow.

Repository geometry

The geometry of the repository can only be very marginally influenced by intact rock deformation. Intact rock deformation can, however, induce deformations along existing fractures and fracturing, which in combination may induce rock fall leading to changes in the shape of the periphery of the excavated rooms.

Fracture and pore geometry

Aperture changes, closure and opening, will take place in response to intact rock deformation. Intact rock deformation may also cause some propagation of fractures, thus changing the network.

Rock stresses

Intact rock deformation causes changes in rock stresses depending on the properties of the rock types and on the boundary conditions.

Matrix minerals

Intact rock deformation does not alter the composition of matrix minerals (not considering extremely long geological time periods).

Fracture minerals

Intact rock deformation will not alter the composition of fracture minerals at the pressures expected in this shallow system.

Groundwater composition

Intact rock deformation will not alter the groundwater composition.

Gas composition

Intact rock deformation will not influence the gas composition.

Structural and stray materials

Intact rock deformation may cause changes in the loads on the reinforcement, in early stages when rock bolt or shotcrete are still active. Rock deformation may also influence the support load for tunnel plugs.

Saturation

Aperture changes, closure and opening, will take place in response to intact rock deformation. Under unsaturated conditions, or if the pore pressure is very low, this could impact on the degree of saturation.

4.2.3 Boundary conditions

The most important boundaries for mechanical processes consist of the far-field horizontal stresses, determined by tectonic loads. At SFR the magnitude of horizontal stresses is larger than the vertical stress. The peripheries of the repository openings and the ground surface are also the boundaries of the geosphere for all mechanical processes. The normal and shear boundary stresses acting on the opening peripheries will both be zero before deposition and backfilling. At the initial state, when the repository is closed, there will be very minor boundary stresses around the excavation openings due to the backfill materials. The ground surface will be at zero normal stress at all times except for the glaciation period, when the boundary normal- and shear stress will vary due to effects of the glacial loading.

4.2.4 Model studies for deformation of intact rock

The process of intact rock deformation is well known and modelling of this process is common. There are models with different degree of simplification, ranging from models assuming isotropic and linearly elastic behaviour to models that includes stress-dependency, anisotropy and plasticity. For large geometrically complex underground constructions such as the SFR, numerical modelling is normally used to analyze the expected mechanical behaviour. Parameter values used as input to model studies that include intact rock deformation are normally based on results of well-established laboratory tests (ISRM 2007).

4.2.5 Natural analogues for deformation of intact rock

The knowledge of intact rock deformation relies on results from laboratory tests. There are different test methods where fairly small intact rock samples are subjected to uni-axial or tri-axial compressive loading, as well as tensile loading tests. During loading up to failure the deformations are recorded. The methods are standardised and described in ISRM (2007).

The effects of intact rock deformation may also be observed at a larger scale during the excavation of tunnels and caverns. However, fracture displacements will often overshadow the intact rock displacements in a rock mass, and the applied loads are uncertain, which make quantitative determination of intact rock properties from field observations difficult.

4.2.6 Time perspective for deformation of intact rock

Deformation of the intact rock will mainly take place during excavation and during the periglacial period. During glacial and post-glacial periods the rock mass will also experience non-negligible changes in rock stresses and, accordingly, some deformation of the intact rock is anticipated.

4.2.7 Handling of deformation of intact rock in the safety assessment SR-PSU

A numerical model study has been carried out specifically for the safety assessment of SFR. This study, presented in Mas Ivars et al. (2014) is a block stability numerical model to demonstrate the overall stability from the rock caverns up to the seafloor above. The model is also used to demonstrate stability of the pillar between caverns. In this model the process of intact rock deformation is a main component. The material properties for the intact rock were based on laboratory tests on samples from Forsmark. Some of the models were made with rigid blocks (i.e. rock properties not needed) and some with deformable intact rock blocks. Intact rock behaviour plays no critical role for the two stability issues studied, and the models with deformable and non-deformable blocks give fairly similar results.

The expected thermo-mechanical effects during the periglacial and glacial periods are not handled in the assessment. The effects are judged to have insignificant effect on the groundwater flow modelling.

4.2.8 Handling of uncertainties

The main uncertainty with respect to intact rock deformation is associated with the uncertainty in the load changes that will occur over the long-term. For example, there is uncertainty in the temperature change that will occur over the life time of the repository and there is uncertainty in the properties of the larger deformation zones, which leads to uncertainty in predicted stress changes. The elastic properties, and the thermal expansion, of the intact rock are fairly well known and the process of deformation of the intact rock is fairly well understood. There is a variation in behaviour for different rock types (SKB 2013b), and this causes an uncertainty in prediction prior to excavations, but this uncertainty will considerably lessen once the rock types are excavated and characterised. The uncertainty of mechanical properties is, however, larger when regarding the rock mass at larger scales, i.e. including both the intact rock and fractures of different sizes.

4.2.9 Adequacy of references regarding deformation of intact rock

The references are judged to be adequate to support the handling in SR-PSU.

4.3 Displacements along existing fractures

4.3.1 General description of displacements along existing fractures

Displacements along existing fractures refer to all reactivation and displacements associated to existing fractures in the rock in the initial state, including elastic movements and irreversible slip. Fracture sizes follows a continuous spectrum (e.g. Fox et al. 2007, Darcel et al. 2009). The smallest fractures, with equivalent radii ranging from µm to dm, are regarded as a constituent of the intact rock. Mesoscale fractures, which are considered here, range in size from some dm up to the size of minor deformation zones. Deformation zones are not included in this assessment as the facilities are purposely designed not to intersect these.

Small fracture samples (50 mm to 200 mm) have been tested in the laboratory to determine properties such as the stiffness and shear strength.

Fracture displacements are described in terms of normal displacement, i.e. opening or closing, and shear displacements, i.e. slip along the fractures. Normal stiffness and shear stiffness are the parameters used in simple models to predict fracture displacements. The stiffness of a fracture is usually stress dependent. The fracture shear strength may be described by a two parameter linear Mohr Coulomb model: cohesion and friction angle, or more elaborate nonlinear models.

4.3.2 Dependencies between displacements along existing fractures and geosphere variables

In this section, dependencies between this process and defined geosphere variables are outlined. Table 4-3 lists how a change in the variables influences the process, i.e. how the change directly influences displacements along fractures. The rightmost column indicates how this influence is handled in the safety assessment SR-PSU. Table 4-4 lists instead how a change in the process directly influences the geosphere variable. After the tables follow for each variable a short paragraph in which the dependency is further described.

Table 4-3. Direct influences of defined geosphere variables on the process "Displacements along existing fractures" and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.3.7).
Temperature in bedrock	No, but indirectly via thermally-induced changes in rock stress.	T/P/G	
Groundwater flow	No.	–	–
Groundwater pressure	Yes.	All	Not handled. Main influence from pressure change is during glaciation. The effective stress is not handled in the models for stability analyses.
Gas phase flow	No.	–	–
Repository geometry	Yes.	All	Geometry is input to stability analyses. See Section 4.2.7.
Fracture and pore geometry	Yes.	All	Fracture size, location and orientation determine the displacement, and are input to stability analyses. See Section 4.2.7.
Rock stresses	Yes.	All	Stress is input to stability analyses. See Section 4.2.7.
Matrix minerals	Yes.	All	Elastic properties, determined by mineral composition, are input to any mechanical analysis.
Fracture minerals	Yes.	All	Estimations of fracture properties in models based on laboratory tests on samples from the area.
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	Yes.	All	The support from structural materials are assumed zero in models of cavern stability. Plug interaction with rock fractures is not handled.
Saturation	No, but indirectly through pore pressure.	–	–

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-3

Temperature in bedrock

Thermally induced stress perturbations may cause different kind of displacement, opening, closing or slip along the fractures. Freezing of the groundwater inside the fracture will also cause a change of the stresses, which may give rise to fracture opening and propagation.

Groundwater flow

Groundwater flow will not influence the displacements along fractures. (Erosion in fractures is discussed as a separate process, Section 4.5).

Groundwater pressure

A change in the groundwater pressure will change fracture effective stresses. This causes the fractures to open or close, accordingly. A change in effective stress also influences the shear stiffness and strength of fractures.

Gas phase flow

Gas phase flow does not influence the displacements along rock fractures.

Repository geometry

The geometry, such as size and shape, of the repository will influence how the stresses are distributed in the rock volume around it. The displacements along the fractures at the repository are thus influenced by the geometry. For example, a large span cavern will have more rock blocks in the zone of stress changes if compared to a smaller span cavern.

Fracture and aperture geometry

The fracture network geometry, the fracture size and the aperture geometry in the fractures has a clear influence on the displacements along the fractures. The orientation of the fracture with respect to rock stresses determines fracture shear- and normal stresses. The degree of match and contact areas between fracture surfaces determine the shear strength, and the angle and connections to other fractures determine the degree of freedom for blocks and fractures to move. The size (area) of the fracture steers the maximum slip that the fracture can host (Eshelby 1957).

Rock stresses

Stress is input to stability analyses (see Section 4.2.7).

Matrix minerals

The composition of minerals determines the deformation properties in the host rock for fractures, which means that the fracture displacements will also be influenced by the differences in matrix materials. The strength of the fracture rock asperities will be a component of the shear strength of a fracture. However, the fracture properties in crystalline rocks are usually dominated by the amount of softer infilling materials and the geometrical properties of the fracture surfaces.

Fracture minerals

Larger amounts of soft minerals in a fracture, such as chlorite and clay, are a common cause of low stiffness and low strength in fractures. Therefore, the type of fracture mineralisation steers the slip potential of the fracture.

Groundwater composition

Groundwater composition does not have any influence on fracture displacement.

Gas composition

Gas composition does not have any direct influence on fracture displacement. The fraction of (reactive) carbon dioxide gas is expected to be small (cf. Section 3.3).

Structural and stray materials

Rock bolts and shotcrete reinforcement are installed in tunnels and rock cavern to inhibit potentially unintended block fall-outs during the excavation and operational stage, i.e. to prevent fracture shear failure and slip. The extent and deterioration of rock reinforcement will thus influence the fracture displacements that takes place around the repository caverns. The backfill in tunnels and cavern may limit the displacements associated with loosened blocks in the wall or roof. Further, at plug locations the rock fractures may be mechanically influenced by the loads from plug materials.

Saturation

Saturation may only influence fracture displacement indirectly through the change in pore pressure when saturation changes.

Table 4-4. Direct influences of the process "Displacements along existing fractures" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.3.7).
Temperature in bedrock	No.	–	–
Groundwater flow	No, but indirectly through fracture and pore geometry.	All	Not handled. H-M coupling are not considered important for safety assessment.
Groundwater pressure	No, but indirectly through fracture and pore geometry affecting groundwater flow.	–	–
Gas phase flow	No, but indirectly through fracture and pore geometry.	–	Not handled. Gas phase flow is very limited.
Repository geometry	Yes.		Changes in the geometry of the excavated rooms due to rock fallout are analysed. Fracture displacements and stress redistribution are output from the stability analysis.
Fracture and pore geometry	Yes.		Not handled. The models assume persistent fractures and fracture propagation is not simulated. Fracture displacement will cause closure or opening in models, but the aperture is not used for flow analyses.
Rock stresses	Yes.		Fracture displacement will cause stress relaxation or stress redistribution in the models. But changes in effective stresses due to changes in pore pressures are not handled.
Matrix minerals	No.	–	–
Fracture minerals	No.	–	–
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	Yes.		Neglected. In the stability analyses the effect of structural material (such as the rock bolts and concrete in the tunnels) is neglected, since the function of support will not remain in the long time perspective.
Saturation	No.	E/O/S	–

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-4

Temperature in bedrock

A displacement along a fracture will not influence the temperature in the rock. Friction work is here neglected. Significant heat would only be produced during major earthquakes.

Groundwater flow

Shear displacements along fractures will normally result in a dilation of the fracture. This means that the aperture, and the aperture distribution, changes and leads to an increased groundwater flow through the fracture. How large this coupling is, between shear displacement and flow increase, depends on the characteristics of the fracture surfaces and fracture boundary conditions.

A displacement along a fracture in the normal direction will take place when the effective stress inside the fracture changes. This could be due to a change in rock stress or due to changes in the pore pressure in the fracture. Such opening or closure of the fracture (i.e. fracture geometry) will of course influence the flow in the fracture accordingly. For the simplified case with two parallel fracture surfaces, it can be shown that the flow Q is proportional to the aperture to the power of three, which means that there is a strong correlation between fracture displacement and groundwater flow.

However, the flow through the rock mass is also determined by the connectivity between fractures and the distribution of fracture infilling material, which is governed by the geological history for each fracture.

Groundwater pressure

Normal displacements will change the groundwater pressure in hydraulically disconnected fractures. However, large fractures in a rock mass are, usually connected to other fractures.

Slow fracture displacements, also assuming that the fracture is connected to other fractures, will not influence the groundwater pressure directly. However, the pressure distribution may be altered if a sufficient number of connected fractures are subjected to displacements, i.e. the boundary condition changes are widespread and sufficiently large.

Gas phase flow

Fracture displacements may influence the gas phase flow indirectly via interactions with fracture and pore geometry (the apertures of the fracture), similar to groundwater flow.

Repository geometry

If there is a major fracture displacement occurring around the periphery of the excavation, such as rock block fallout, the geometry at this point will of course change and the stresses will redistribute in accordance with the new geometry. Most geometry changes due to displacements will however be negligible small, in the order of a few mm. An earthquake scenario could possibly give rise to shear displacements in the order of several cm.

Fracture and aperture geometry

Displacements of existing fractures will directly have an influence on the fracture geometry, in the sense that the aperture, and the aperture distribution, will change (See groundwater flow above). The geometry of the fracture network will remain unchanged, as long as no major propagation and coalescence of fractures takes place.

Rock stresses

Fracture displacements will cause stress changes around the fracture. Points on the fracture surface that may have previously transferred load to the other side may no longer be in contact, and vice versa. The stresses at the fracture tips will change if a fracture is sheared. The scope and extent of the impact on stresses depends on the nature and the magnitude of the displacement.

Matrix minerals

Fracture displacements do not influence matrix minerals.

Fracture minerals

With the notable exception of seismic slip, that may produce pseudotachylate, fracture displacements do generally not influence the type of fracture minerals, but could degrade or deform the material.

Groundwater composition

Fracture displacements do not influence groundwater composition.

Gas composition

Fracture displacements do not influence gas composition.

Structural and stray materials

Fracture displacements may alter the load on rock bolts if intersected by the fracture and change the load on shotcrete reinforcement. In the long term perspective, the support of the construction is lost. This was also an assumption in the stability analyses by Mas Ivars et al. (2014).

Further, a displacement of fractures close to a plug construction could change the pressure, or the properties of the contacts, against the plug components.

Saturation

Fracture displacements do not influence the saturation of the rock mass.

4.3.3 Boundary conditions for models regarding displacements along existing fractures

See Section 4.2.3.

4.3.4 Model studies of displacements along existing fractures

Model studies made to analyze rock stability problems generally include a model for the fracture displacements. There are different constitutive models used to describe the fracture displacement mechanisms. The most common failure criterion is the Coulomb slip model, which is defined by cohesion and a friction angle.

The elastic displacement is often modelled by a constant stiffness value, but also stress-dependent stiffness models are used. A conscious selection of normal stiffness in the analyses may well be important, since the normal stiffness is strongly stress-dependent. This is illustrated in Figure 4-1 which shows a typical result from a normal stiffness and shear laboratory test, on a small fracture sample.

The knowledge of fracture behaviour is based on laboratory testing on small samples, and the certainty in mechanical parameters is less for larger fractures. Also, a large spread in behaviour between different types of fractures, i.e. fractures with different geological history having different geometrical and mineralogical characters, should be expected. The estimations made for fractures model parameters at the SFR are given in SKB (2013b).

4.3.5 Natural analogues for displacements along existing fractures

The quantitative knowledge on fracture strength and stiffness is mainly based on laboratory studies on small samples. However, the mechanisms of fracture displacements are commonly observed in connection with rock constructions and mining. A natural example of where fracture displacements may be observed is at rock slides in steep unstable rock slopes. On a larger scale, fracture displacements (reactivation) may also be studied as a result of earthquakes.

4.3.6 Time perspective for displacements along existing fractures

Displacements along existing fractures will mainly take place during excavation as a response to stress redistribution around the tunnels and caverns. During the periglacial period freezing of ice inside fractures will cause the fractures to dilate and possibly propagate. Creep in fractured rock should be expected to some limited but unknown extent since stress levels are low compared to rock strength (see process fracturing Section 4.3.3). Fractures may slip as a response to nearby earthquakes, the frequency of which scales with time as shown in Bödvarsson et al. (2006).

4.3.7 Handling of displacements along existing fractures

For many engineering problems regarding rock masses the most important and dominating mechanical process is the displacements (reactivation) along the existing fractures, and it is judged that this is the case also for the SFR facility. The handling of this process in the safety assessment for SFR is presented in the following sections.

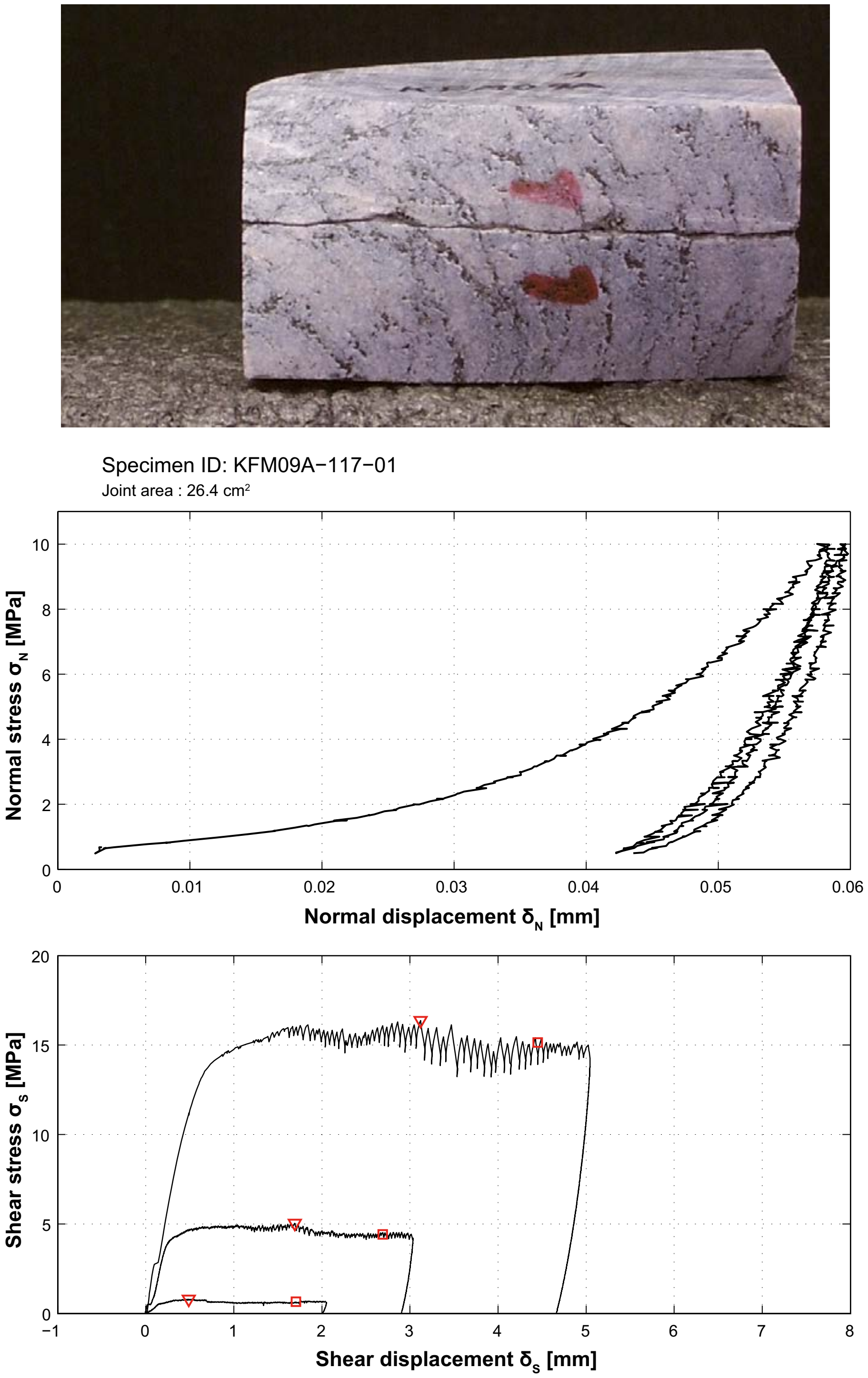

Figure 4-1. *Typical results from a test on a small fracture sample from the Forsmark site investigation (Jacobsson and Flansbjer 2006). The upper diagram shows results from a normal loading text with two loading and unloading cycles. The slope of the latest cycle is used to determine the normal stiffness. The lower diagram shows shear-displacements curves from a shear test. The different colours refer to repeated shearing at different normal load on the sample during shearing. The initial curve slope determines the shear stiffness and the shear stress level at the plateau gives the shear strength.*

Issue of stability in the rock mass above and between SFR caverns

A numerical study analyzing the long term stability of the rock caverns at SFR-1 has been performed, and is presented in Mas Ivars et al. (2014). This study had two objectives: to analyze if there is a risk for loosening of the rock up to the surface and if there is a risk for instability in the pillars between caverns.

Numerical models were built using 3DEC (Itasca 2011), which is a three-dimensional discrete element program which means that the rock mass is simulated as an assemblage of rock blocks with fracture elements between the blocks. The study was based on simplifications and assumptions described in the following.

Two caverns, BLA and BMA were included in the three-dimensional numerical model. Cavern BLA is not backfilled at all in the model, and in the BMA model the space between the concrete cap and the roof of the cavern is not backfilled. These are strongly conservative assumptions compared to the actually planned degree of filling (SKB 2013b).

Eight geometrically different models, using different Discrete Fracture Network model realisations from the same 3 fracture sets, have been analysed (Mas Ivars et al. 2014). The blocks in these models are deformable. The fractures in the models are all persistent and extend through the whole model. Assuming all fractures to extend through the model is a conservative simplification but disregarding the effect of random fractures, and the limited number of analysed cases is not conservative.

Two models with rigid blocks were also analysed. In the first case the fracture sets were used with a constant strike and dip, and in the second case the fractures were generated with a variation in orientation. The reason for carrying out these two analyses with rigid blocks was that the calculations becomes much faster, and therefore it was practically possible to study the caving process to the end in these cases.

The groundwater pressure in the model is not explicitly simulated in the model. The model is purely mechanical and the model does not handle the effective stress or the hydro-mechanical coupling. This was a necessary model simplification, which is not conservative. The strength properties of fractures are lowered when the water pressure inside the fractures and the effect of water on the fracture surface are considered. However, a way to indirectly take this effect into account in the analysis is to adopt lower strength properties (i.e. lower friction angle), to a corresponding degree, in the purely mechanical model.

The degradation of the fracture strength with time is simulated by reducing the fracture friction angle and cohesion, in steps, down to very low values, and more in the area closer to the caverns. The results from the simulations show that blocks around the excavation boundaries become unstable and start falling into the cavern when the friction angle is reduced from 25° down to 5.7°, for the in situ stress case assumed. This is a friction angle which is clearly lower than what is expected for the vast majority of fractures at the site.

The results for the case with low in situ stress show that block fallouts starts when the friction angle is reduced to 18.2° (See Figure 4-2). The stability is quite sensitive to the assumed in situ stress. For the case with stress magnitudes as predicted in SDM-PSU (SKB 2013b), the caverns are stable.

In rigid block model cases where the blocks are allowed to fall into the cavern the caving process stops after the empty space is filled with blocks. The height of the loosened rock mass reaches at this stage up to 34 m above the roof, and above this level a stable arch is formed, and the caving does not in any analysed case continue up to the sea floor. This means that there should be no risk, within the already acknowledged uncertainties, that a direct connection between the caverns and the seafloor will develop.

The numerical analyses by Mas Ivars et al. (2014) also predict that the pillar between the two caverns BLA and BMA of the model is stable in all studied cases.

No stability analysis has been performed specifically for the extension of SFR. This part of SFR is, however, planned to be located deeper than SFR-1, which is advantageous for the stability around the caverns. The geometry and orientation of caverns and the geological conditions are predicted similar for the extensions compared to the existing SFR (SKB 2013b).

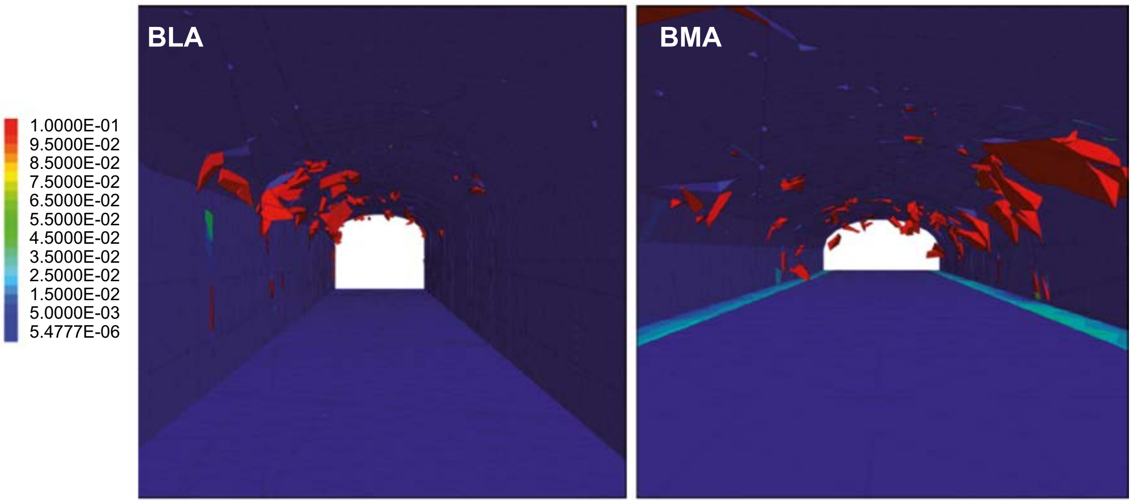

Figure 4-2. *View of the caverns with displacement contours (in m) once the critical fracture friction angle 18.2° has been reached, for a case with hydrostatic stress (Mas Ivars et al. 2014).*

The mechanical effect from an earthquake scenario has not been calculated within the safety assessment of SFR. The consequence of an earthquake is expected to be displacements along fractures. But, as shown above, an overall stability of caverns and pillars is foreseen even for a situation where rock blocks start loosening around the excavations.

Issue of damage of technical barriers

According to SKB (2013b) the rock caverns will be fully filled with backfill material, which will prohibit extensive rock fall-outs. Also, in the silo there will be a thick concrete slab molded on top of the waste compartments such that even rock fallouts would not damage the concrete structure.

The effect on the concrete structure due to rock load is not handled in the analyses of earthquake load effects on the silo concrete structure (Georgiev 2013). It is assumed that such loading from rock would be small in comparison with the total weight of the structure, and the effect is therefore neglected in the analyses.

4.3.8 Handling of uncertainties

The main uncertainty with regard to fracture displacements is the mechanical properties used in the modelling of the displacements. Fracture properties are currently obtained from mm-scale laboratory tests. Fracture displacement predictions are required for large scale fractures. The uncertainty in the large scale properties and their variability compared to the laboratory properties is unknown. Nevertheless, if the load changes can be foreseen and quantitatively estimated, it is judged that the current understanding of rock fracture properties is sufficient to make conservative analyses.

4.3.9 Adequacy of references regarding displacements along existing fractures

The references are judged to be adequate to support the handling in SR-PSU.

4.4 Fracturing

4.4.1 General description of fracturing

Fracturing implies the creation of new fractures in intact rock and/or the propagation of existing fractures into intact rock. Fracturing is a non-reversible process in contrast to elastic displacements. The kind of time-dependent deformation and fracturing, that occurs as a result of long-term exposure to high levels of stress, if often denoted creep. Creep is here not treated as a separate mechanical process.

4.4.2 Dependencies between fracturing and geosphere variables

In this section, dependencies between this process and defined geosphere variables are outlined. Table 4-5 lists how a change in the variables influences the process, i.e. how the change directly influences deformation of intact rock. The rightmost column indicates how this influence is handled in the safety assessment SR-PSU. Table 4-6 lists instead how a change in the process directly influences the geosphere variable. After the tables follow for each variable a short paragraph in which the dependency is further described.

Table 4-5. Direct influences of defined geosphere variables on the process "Fracturing" and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.4.7)
Temperature in bedrock	No, but indirectly though rock stress.	–	–
Groundwater flow	No.	–	–
Groundwater pressure	Yes.	All	Not handled. The influence considered negligible to safety assessment.
Gas phase flow	No.	–	–
Repository geometry	Yes.	All	Not handled. The influence considered negligible to safety assessment.
Fracture and pore geometry	Yes.	All	Not handled. The influence considered negligible to safety assessment.
Rock stresses	Yes.	All	Not handled.
Matrix minerals	Yes.	All	Rock types are given different strength properties in the models performed.
Fracture minerals	No, but indirectly through fracture strength and fracture displacement.	–	–
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	Yes.	All	Not handled. The effects are considered negligible since the materials is assumed to be degraded (cf. Section 5.8) i.e. cautious assumptions in the SR-PSU assessment.
Saturation	No, but indirectly through pore pressure.	–	–

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-5

Temperature in bedrock

A temperature change will cause deformation of the intact rock, and this may change the stress situation such that fracturing is influenced. Also freezing could lead to fracturing due to pressure from expanding ice in fractures. But there is no direct coupling between temperature and fracturing.

Groundwater flow

Groundwater flow has no influence on rock fracturing.

Groundwater pressure

Groundwater pressure determines the effective stress in the bedrock, and is thus a factor that can influence the fracturing process. In particular when the normal total stress is low a change in pore pressure may be of significance for fracturing.

Gas phase flow

Gas phase flow has no influence on rock fracturing.

Repository geometry

The shape and size of the repository tunnels and caverns will determine how the stresses are distributed in the rock around excavations. Therefore the geometry has an influence on which areas will experience some fracturing. For example, the risk for spalling mechanisms to occur is different depending on the orientation and height of caverns.

Fracture and pore geometry

The intensity of fractures and the orientation of fractures have a clear influence on if, and how, fracturing takes place in a rock mass. A rock mass with high fracture frequency, persistent fractures in a strong rock will be clearly less prone to fracturing compared to a weaker rock with few short fractures. In the first case almost all deformations will be taken in the existing fractures and no new fractures are needed to respond to load changes, while in the second case propagation of existing shorter fractures may be needed to connect to other fractures or the intact rock will experience stresses higher than its strength and fail with new fractures forming.

Rock stresses

The level of stress determines the extent of the fracturing process. The criteria on the stresses to cause a fracturing process is described, and simplified, using different material models. The strength model often used for intact rock is the so called Mohr–Coulomb material model. Material parameters describing the predicted strength of rock types at SFR are found in SKB (2013b).

Matrix minerals

The different matrix minerals of the different rock types occurring, and the grain size of the minerals, are factors that determine the strength. Geological description of the different rock types and predictions of mechanical properties are found in SKB (2013b).

Fracture minerals

The minerals inside the fractures will not directly influence the fracturing. However, since the infillings influences fracture displacement, which gives stress changes around the fracture, there is an indirect coupling to fracturing.

Groundwater composition

Groundwater composition does not influence the fracturing process.

Gas composition

Gas composition does not influence the fracturing process.

Structural and stray materials

The load that is applied to the rock walls from structural materials, such as the concrete plugs, may have an influence on the potential for fracturing in the rock at these points. However, as rock enforcement is assume to be degraded (cf. Section 5.8) the effect is negligible.

Saturation

The saturation of the repository will not have any influence on the fracturing, other than indirectly through the pore pressure and effective stress.

Table 4-6. Direct influences of the process "Fracturing" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.4.7).
Temperature in bedrock	No.	–	–
Groundwater flow	No, but indirectly through fracture and pore geometry.	All	–
Groundwater pressure	No, but indirectly through groundwater flow, fracture and pore geometry.	–	–
Gas phase flow	No, but indirectly through fracture and pore geometry.	All	Not handled. Both fracturing and gas phase flow is very limited.
Repository geometry	Yes.	All	Not handled. The influence considered negligible to safety assessment.
Fracture and pore geometry	Yes.	All	Not handled. The glacial phase is not modelled. The influence on plugs is assumed negligible.
Rock stresses	Yes.	All	Not handled. The models assume elastic material model. The fractures are assumed to dominate and with conservative properties.
Matrix minerals	No.	–	–
Fracture minerals	No.	–	–
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	Yes.	–	Not handled. The rock is approximated to be intact (elastic) and impermeable at the plugs. The importance of EDZ for SFR performance is of potential significance only in connection to hydromechanical processes at the plugs. For handling of this issue refer to the **Barrier process report**.
Saturation	No.	–	–

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-6

Temperature in bedrock

Fracturing does not have any influence on the temperature.

Groundwater flow

Fracturing will increase the hydraulic conductivity of the rock. How strong this coupling is depends largely on the circumstances, such as confining stresses and the properties of already existing fracture network.

Groundwater pressure

Fracturing will not directly influence the groundwater pressure, but indirectly through the groundwater flow.

Gas phase flow

Fracturing will increase the permeability of the rock, and thus increase the possibilities for gas phase flow.

Repository geometry

Fracturing could in some cases, when part of an instability situation, influence the geometry of a cavern periphery. To become significant this process should take place in combination with displacement and failure along existing fractures.

Fracture and pore geometry

Fracturing will, by definition, influence the fracture geometry. Fracturing increases the fracture intensity and increases the pore volume, at least at the points where it is occurring.

Rock stresses

Fracturing clearly influences the stresses. At a point where fracturing occurs the stresses built up are released and the stresses redistribute until a new equilibrium state is gained.

Matrix minerals

Fracturing has no influence on the matrix minerals.

Fracture minerals

Fracturing has no influence on the fracture minerals.

Groundwater composition

Fracturing has no influence on groundwater composition.

Gas composition

Fracturing has no influence on gas composition.

Structural and stray materials

Fracturing has in general no significant influence on the structural materials. A potential exception to this would be that a failure in the rock at the support for a concrete plug construction. Such fracturing could lead to deformations in the rock that in turn influences the stresses and deformations in the plug. The loads in a plug depend on its design (SKBdoc 1346127).

Saturation

Fracturing does not influence the saturation in the repository.

4.4.3 Boundary conditions for models regarding fracturing

See Section 4.2.3.

4.4.4 Model studies of fracturing

The progressive failure of intact rock has been studied by many researchers. There is a common understanding of how micro cracks grow and finally coalesce into macro-scale fractures. Based on extensive laboratory testing on rock samples several constitutive models for the fracturing process have been presented. In the numerical models that have been used for analyzing rock mechanics problems the way to incorporate fracturing depends on the type of approach (Jing 2003).

The most simple and common way to analyze fracturing is to just postulate a condition on the stresses, that is seen as limiting for fracturing to start, and that the fracturing itself is not modelled. The criterion is then most often put on the deviatoric or shear stress, such as when using the Mohr–Coulomb failure criterion, based on laboratory results. The shear stress in these models cannot increase above a certain value and the failure process is simulated through some constitutive model like plasticity. This type of modelling will indicate if there is a risk for fracturing and in which areas this is to be expected.

There are also numerical programs that aim at simulating the fracturing process itself, using boundary element methods (e.g. Backers et al. 2012, Shen et al. 2014) or discrete element methods (e.g. Potyondy 2012, Cai et al. 2007). When using this kind of program a criterion is postulated on the stress conditions at the tip of the already existing fracture tips in the model. If the propagation criterion is met the model will simulate an incremental growth of the fracture from the tip in the direction calculated and then continue calculating the stress redistribution for next step in the analysis.

4.4.5 Natural analogues for fracturing

Rigorous experimental studies of rock fracturing in the actual scale are almost impossible to perform due to the large scales and the loads needed. But observations of natural fracturing and fracturing at underground excavations are of course commonly studied within rock mechanics research. However, the geometrical properties as well as the loading situation are normally hard to determine with any accuracy in the in situ conditions. The process of fracturing is closely coupled to the process of deformation of the intact rock and the displacements along fractures, which further adds to the complexity.

The ground condition that is expected to cause most fracturing in the SFR facility is fracturing due to the freezing process inside existing fractures, in the periglacial and glacial time periods. Fracturing due to freezing has been studied both theoretically and in the laboratory and field (Tharp 1987, Wegmann and Gudmundsson 1999).

Observations in the field are mainly done in connection with studies of rock slopes and free walls. The situation with a submerged backfilled tunnel will be different from that of a rock slope. Such fracturing process might be studied in mines located in periglacial regions, such as the Lupin Mine.

4.4.6 Time perspective for fracturing

See Section 4.2.6.

4.4.7 Handling of fracturing

Fracturing processes are not directly handled in the safety assessment. Scenarios where fracturing is judged to be present have been evaluated without simulating fracturing. Instead of simulating the fracturing process, fracture trace lengths are increased. The model analyses performed in Mas Ivars et al. (2014) has been selected conservatively by representing the fractures with large persistence, which means that the creation of new fractures, through propagation/fracturing, is not needed to simulate a potential lowest strength case around the caverns.

It is possible that the excavation of the caverns has resulted in an Excavation Damage Zone (EDZ) due to fracturing. This zone will then be part of the initial state for the repository. The influence of an EDZ that results from modern day excavation methods is judged to be of no relevance to large scale stability that influences long-term safety. The importance of EDZ for SFR performance is judged only of potential significance in connection to hydro-mechanical processes at the plugs. For handling of this issue refer to the **Barrier process report**.

After the initial state, it is only during the freezing and thawing periods that a fracturing process at the rock excavation boundaries is expected. This process is not explicitly included in the safety assessment because the additional fracturing of the rock is not expected to significantly influence the groundwater flow during the periglacial or glacial period. A safety assessment scenario, in which there is no retention in the geosphere is however included in SR-PSU.

4.4.8 Handling of uncertainties

Fracturing in a rock mass is a complex process and a function of in situ stresses, rock types, anisotropic textures and geometry of the natural fracture network. Consequently any fracturing model is an idealised simplification. The main uncertainty lies in this simplification process.

The most likely scenario that will cause fracturing is during the periglacial period with water freezing inside the rock fractures. This may cause existing fractures to propagate. However, there is considerable uncertainty in the understanding of how freezing-induced fracturing will develop in the repository.

4.4.9 Adequacy of references regarding fracturing

The references are judged to be adequate to support the handling in SR-PSU.

4.5 Erosion and sedimentation in fractures

The process of erosion and sedimentation in fractures depends mainly on two factors, the driving forces from the groundwater and the resistant force through the strength of the material in the fracture. The driving force from the groundwater flow is determined by the groundwater pressure gradients. During excavation and operation of the repository facility the local hydraulic gradient will be high close to the rock tunnels and caverns, while the hydraulic gradients after repository closure will be governed by the variation in surface elevation, and which can be emphasised by the passage of an ice front. The general mechanisms of erosion and sedimentation, and studies performed on the force from the groundwater and the strength of fracture filling/gauge are further described in SKB (2010e).

4.5.1 Dependencies between erosion and sedimentation in fractures and geosphere variables

In this section, dependencies between this process and defined geosphere variables are outlined. Table 4-7 lists how a change in the variables influences the process, i.e. how the variable change directly influences erosion and sedimentation in fractures. The rightmost column indicates how this influence is handled in the safety assessment SR-PSU. Table 4-8 lists instead how a change in the process directly influences the geosphere variable. After the tables follow for each variable a short paragraph in which the dependency is further described.

Explanation of Table 4-7

Temperature in bedrock

Temperature changes do not have any direct influence on the process of erosion and sedimentation.

Groundwater flow

Groundwater flow is what causes the erosion to take place. High levels of flow are needed to achieve a major erosion process. The groundwater flow gives drag shear forces from the water to the material in the fracture. When the shear forces are sufficiently high the erosion process will start.

Groundwater pressure

Groundwater pressure does not directly influence the erosion, but the pressure gradients will determine the groundwater flow (see above).

Gas phase flow

Gas phase flow is not a factor for the process of erosion and sedimentation in fractures, since the amount of gas flow is so limited.

Table 4-7. Direct influences of defined geosphere variables on the process "Erosion and sedimentation in fractures" and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.4.7)
Temperature in bedrock	No.	–	–
Groundwater flow	Yes.	All, but mainly E/O/G	Neglected. Grouting is applied during construction and the shear forces from water flow are expected too low for natural gradients to cause erosion.
Groundwater pressure	No, but indirectly strong influence through groundwater flow.	–	See above.
Gas phase flow	Yes.	All	Neglected. No sufficiently strong gas flow is expected.
Repository geometry	No, but indirectly through location with different fracture and pore geometry.	–	–
Fracture and pore geometry	Yes.	All	Neglected. The shear forces are too low to cause any significant erosion. (See groundwater flow.)
Rock stresses	No, but indirectly through fracture aperture and groundwater flow.	–	–
Matrix minerals	Yes.	All	Neglected. The bonding strength is larger than erosive force.
Fracture minerals	Yes.	All	Neglected. The shear strength of filling materials is much higher than expected shear forces.
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	Yes.	All	Neglected. The shear forces are expected to low to cause significant erosion or sedimentation of structural material.
Saturation	Yes.	All	Neglected. Both gas flow and groundwater flow shear forces are too low.

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Repository geometry

The repository geometry does not directly influence the erosion, but indirectly since the location (for example the depth) of the repository gives intersection with different fractures having different infilling materials and pore geometry.

Fracture and pore geometry

The fractures aperture and the pore geometry that is important for the process of erosion. It is the fracture with larger apertures hat will be mainly subjected to the flows needed.

Rock stresses

Rock stresses does not directly influence the process of erosion, only indirectly through aperture changes.

Matrix minerals

Negligible influence. The bonding strength of the matrix minerals is larger than the erosive force.

Fracture minerals

The mechanical properties and the location of the fracture infilling is a main factor determining if erosion will take place or not. Loose infillings, such as clay or gauge, are more prone to erode.

However, there will also be instances when closely packed clay size minerals will be difficult to erode. And very fine clays will also be difficult to move as they will be attracted by sub-atomic forces at the mineral edges.

Groundwater composition

Groundwater composition influences the erosion and the sedimentation in fractures only indirectly, by dissolving and precipitating fracture infillings and therefore affecting their properties and the erosion. Higher salinity waters will for example flocculate the clay sized particles and the fresher the water, the more easily will these clay size minerals deflocculate.

Gas composition

Gas composition does not influence the erosion or the sedimentation in fractures.

Structural and stray materials

The grouting performed will be an important measure to decrease groundwater flow during the excavation. This structural material will therefore have a mechanical and chemical influence on the potential for erosion and sedimentation in the fractures.

Saturation

The saturation may have an influence on the erosion and sedimentation in the vadose zone. However the process is neglected since the flow shear forces during periods with unsaturated conditions are judged too low.

Table 4-8. Direct influences of the process "Erosion and sedimentation in fractures" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event*	Handling of influence in safety assessment (see also Section 4.5.7).
Temperature in bedrock	No.	–	–
Groundwater flow	No, but indirectly through fracture and pore geometry.	All	
Groundwater pressure	No, but indirectly through groundwater flow, fracture and pore geometry.	–	–
Gas phase flow	No, but indirectly through groundwater flow, fracture and pore geometry.	All	
Repository geometry	No.	–	–
Fracture and pore geometry	Yes.	All	Not handled. The process is considered negligible within the assessed time period.
Rock stresses	No.	–	–
Matrix minerals	No.	–	–
Fracture minerals	Yes.	All	Not handled. The process is considered to have small influence within the assessment time period.
Groundwater composition	No.	–	–
Gas composition	No.	–	–
Structural and stray materials	No.	–	–
Saturation	No.	–	–

*) E/O/S = Excavation, operation and saturation period, T = temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Explanation of Table 4-8

Temperature in bedrock

Erosion or sedimentation has no effect on the temperature in the rock.

Groundwater flow

If erosion takes place, this will have an influence on the flow in the fracture because the aperture to some extent will increase. If the eroded material does not get trapped and block the flow paths the fracture transmissivity will increase with the erosion process. On the contrary sedimentation in a fracture will lead to a decreased groundwater flow.

Groundwater pressure

Erosion or sedimentation in fractures will influence the distribution of the groundwater pressure in the fractures.

Gas phase flow

As for groundwater flow, erosion or sedimentation process will influence the gas flow, but the amount of flowing gas will not be influenced.

Repository geometry

Erosion or sedimentation has no influence on the repository geometry.

Fracture and pore geometry

The definition of erosion and sedimentation in fractures is that the pore geometry in the fracture is changing. Erosion means that materials are transported with groundwater out from the fracture and sedimentation that material is placed inside the fracture. The fracture network geometry is, however, not changing due to erosion.

Rock stresses

Erosion and sedimentation is expected to occur locally and with limited extent. Erosion will therefore not have any effect on the rock stresses.

Matrix minerals

Erosion or sedimentation has no influence on the matrix mineral composition.

Fracture minerals

Erosion and sedimentation involves changes in fracture mineralogy and composition.

Groundwater composition

To a limited extent there will be changes in groundwater composition due to the dissolution/precipitation of infilling and gauge material associated to sedimentation and dissolution processes.

Gas composition

The erosion or sedimentation process will not change the gas composition.

Structural and stray materials

Structural and stray materials are not influenced by erosion or sedimentation in fractures.

Saturation

Erosion or sedimentation will not change the saturation, at least not after the saturation period of the repository.

4.5.2 Boundary conditions for models regarding erosion and sedimentation in fractures

The boundary condition of importance for the process of erosion and sedimentation in fractures is the groundwater table. The groundwater table determines how high the pressure is and hence governs the hydraulic gradient and the groundwater flow condition. The stress conditions will determine the potential for fracture displacements and aperture increase, which is also a factor that could influence the groundwater flow and the potential for erosion in fractures.

4.5.3 Model studies of erosion and sedimentation in fractures

No model studies have been performed to study the process of erosion and sedimentation specifically for SFR. The process of glacially induced hydraulic jacking (i.e. significant fracture opening) which is needed to have a major erosion or sedimentation is however analysed and discussed in Lönnqvist and Hökmark (2010). More discussion about erosion in fractures may also be found in SKB (2010a).

4.5.4 Natural analogues for erosion and sedimentation in fractures

Erosion and sedimentation in fractures is a natural process that has already taken place at Forsmark (and is observed worldwide). This is seen from the existence of open fractures filled with sediment material that has been transported into the fractures (SKB 2011).

4.5.5 Time perspective for erosion and sedimentation in fractures

Erosion and sedimentation in fractures is mainly expected to happen in connection with the passage of an ice front. This is the time period with the highest groundwater gradients and the period when there could be more significant opening of the subhorizontal fractures close to the ground surface.

4.5.6 Handling of erosion and sedimentation in fractures

The issue of erosion and sedimentation in fractures is not handled in the safety assessment, because it is a process that is mainly expected during a glacial period. Based on current scientific knowledge, the glacial climate domain is not present in the climate cases that support the SR-PSU reference evolution, as described in Section 4.1.2. The possible impact of ice-sheet growth and decay on the repository safety functions is covered by a safety assessment scenario that assumes completely degraded concrete barriers and no geosphere retention (**Climate report**, Section 1.2, and **Main report**, Chapter 7).

4.5.7 Handling of uncertainties

The uncertainty, concerning to what depth and to what extent there will be erosion and sedimentation in the fractures in the future, is quite large. However, there is a high certainty that there will not be any significant erosion or sedimentation taking place during the time period before the next glacial period.

4.5.8 Adequacy of references

All references are to openly accessible articles or from SKB report series.

5 Chemical processes

5.1 Introduction

All processes that are not strictly thermal, hydraulic or mechanical are addressed in this chapter. In that sense the title "chemical" is somewhat misleading. Some processes, such as microbial activities, are clearly not only chemical, whereas other processes are at the borderline between physics and chemistry, such as earth currents. Specific aspects concerning radionuclide migration are discussed in Chapter 6.

Future geochemical conditions will be influenced by the future evolution of climate and climate-related conditions. For instance, shoreline displacement and permafrost development will influence groundwater flow and chemistry, which in turn will affect the geochemical and microbial activities in the geosphere.

The SR-PSU reference evolution, defined on basis of current scientific knowledge, includes periods of temperate and periglacial climate domain (**Climate report**, Section 1.3). In the reference evolution, the future climate development is given by two climate cases, the *global warming* and *early periglacial* climate cases, representing prolonged interglacial conditions at Forsmark due to the combination of an enhanced greenhouse effect and future variations in insolation during the next 50,000 years (**Climate report**, Chapter 4).

In the *global warming climate case,* Forsmark is located in a temperate climate domain for the initial 50,000 years. The period from 50,000 years to 100,000 years after present is defined to describe natural climate variability during a period of global cooling, here represented by a succession of periods of a few centuries to almost 10,000 years of periglacial and temperate climate domain. The *early periglacial climate case* is defined as a variant of the *global warming climate case,* representing the lower end of the uncertainty range associated with the amount of human and natural carbon emissions. Due to a faster temperature decrease in this climate case, a period of periglacial climate domain is defined to occur in the period of minimum summer solar insolation at high northern latitudes from 15,500 to 18,500 years after present.

During the initial period of temperate climate domain in the reference evolution, shoreline migration leads to a terrestrial surface above the repository from a few thousand years after closure and thus increased influence of meteoric water on the rock domain. Further, high-saline groundwater from deeper parts (SKB 2013b) will not influence the groundwater. Thus, low salinity groundwater will prevail during this initial period of temperate climate domain.

In the periods of periglacial climate domain, a lower ground temperature and permafrost conditions are expected. This temperature change and the freezing process of the groundwater will lead to a slow down of chemical reactions and a significant decrease of input of organic matter with recharge waters, giving limited conditions for biogeochemical interactions.

The glacial climate domain is not present in the climate cases that support the SR-PSU reference evolution. However, to span the uncertainty in the timing and duration of ice-sheet growth in the Northern Hemisphere, and for comparison with earlier safety assessments for the SFR repository, a climate case representing a repetition of conditions reconstructed for the last glacial cycle is included in SR-PSU. The *Weichselian glacial climate case* serves to illustrate the possible impact of ice-sheet growth and decay on the repository safety functions (**Climate report**, Section 1.2).

5.2 Advective transport/mixing of dissolved species

5.2.1 Overview/general description

Solutes can be transported through the geosphere by advection and diffusion. Diffusion is described in Section 5.3), while Section 6.2 describes the overall handling of radionuclide transport in the water phase.

Advection

Advection refers to the transport of a dissolved substance by the bulk flow of water. The evolution of the groundwater flow conditions in the geosphere will therefore have a direct and important impact on advective transport. Groundwater flow is diverted to paths with relatively low flow resistance. Therefore, the abundance and properties of rock fractures are important, such as their widths, porosities and connectivities. While local groundwater flow is driven by pressure gradients, it is also affected by the density and viscosity of the fluid. The process of groundwater flow is further described in Section 3.2.

Advection is likely to be the dominant transport mechanism in the geosphere, although solute transport models include both advection and diffusion. The relative importance of the two mechanisms can be evaluated by means of the dimensionless Péclet number, which is the ratio of the rates of these two transport mechanisms. The Péclet number will vary between different parts of the geosphere, for example, advection is likely to dominate in fractures, while diffusion is likely to control solute movement in the rock matrix. However, as the fracture mineralogy changes over time and in response to the biogeochemical conditions, the hydraulic properties of the fractures will change. Therefore, the relative rates of advective and diffusive transport may change over time. See e.g. Bird et al. (2007) for more in-depth theory and descriptions of advective mass transport and related processes.

During the operational period, the zone of low pressure created by the pumping of the repository will draw water inwards (see Section 3.2). When pumping ceases and the repository is being saturated, the advective transport will be directed from the surrounding rock into the repository, and hence dissolved species emanating from the waste forms are not expected to be discharged through the barriers to the geosphere.

Following this initial period, when the vaults, barriers, backfill, and waste packages have become saturated with groundwater, the extent and direction of advective transport of substances is governed by their dissolved concentrations and the local water flow field. The engineered barrier systems of SFR are designed to limit advective transport of materials from the BMA and Silo into the geosphere.

Climate changes during the first 1,000 years of repository post-closure are not expected to affect temperature to any significant degree; therefore no important temperature induced changes with influence on advective transport are expected. However, during periods of permafrost, and perhaps glaciation, the temperature will decrease to a point where the groundwater will freeze to repository depths, or deeper, and water flow and solute transport in the vicinity of SFR will be substantially decreased, see Section 3.2.

Hydrodynamic dispersion

The transport of solutes by advection is also affected by hydrodynamic dispersion, which refers to the net effects of variations in the flow field, in combination with molecular diffusion and mechanical mixing. Dispersion results in a spread of dissolved substances relative to the advective bulk flow of water, and can occur both in the direction of flow and perpendicular to the flow direction. The dispersion effect is caused by different processes such as:

- velocity distribution in single flow channels,
- mixing of water transported by different flow channels,
- distributed flow channel sizes leading to different velocity distributions in different flow channels,
- the presence of materials with different hydraulic conductivities giving rise to distributed flow velocities in different materials, and
- the effects of diffusion processes caused by Brownian motion of dissolved substances in the water.

In a single flow channel, typically the highest velocity is found in the centre of the flow channel and a velocity approaching zero near the channel wall. In materials with distributed channel sizes, the velocity distribution in each of the channels will be different, with the highest velocities expected in the largest channels. When materials with different hydraulic conductivities are present and water flow is parallel to the interface between the different material boundaries, the water flow will be distributed essentially in proportion to the hydraulic conductivity. For flow perpendicular to the material boundaries, the flow will be essentially equal in the different materials, governed by the least permeable material, and the impact on the dispersion processes will be small.

In solute transport modelling, dispersion effects are often represented mathematically by a dispersion factor, which intends to capture the dispersive effects on scales beneath that modelled explicitly by the flow field. Dispersion is sometimes represented using a Fickian approach in modelling, assuming diffusion-like behaviour (see Section 5.3) with a flux proportional to the gradient in solute concentration. However, this approach is not necessarily accurate because it does not explain the observed scale-dependency of dispersivities. Quantifying dispersion for inclusion in simplified advection–dispersion transport models may therefore involve conceptual uncertainties.

5.2.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-1 outlines how the process is influenced by other geosphere variables, while Table 5-2 outlines how the process influences the defined geosphere variables. The influence between the process and each geosphere variable is elaborated upon below.Furthermore it is indicated during what time period, climate domain, or event that the described influence is considered. The handling in the safety assessment SR-PSU for the excavation, operation, and saturation period as well as during the different climate domains is indicated in the rightmost column in the table. In Section 5.2.7, the handling for all time periods, climate domains, and events is discussed by the SR-PSU team.

Explanation of Table 5-1

Temperature in bedrock

No direct influence is identified. Temperature affects the advective transport and mixing of dissolved species indirectly via changes in groundwater flow. Temperature affects groundwater flow through its effect on the density and viscosity of the water, and density differences drive thermal convection. Also, the low temperatures during periglacial climate conditions will affect the aggregation state of water (freezing), see Section 2.2.

Groundwater flow

The extent of advective solute transport is proportional to the magnitude of groundwater flow which therefore has a direct influence on advection.

Groundwater pressure

No direct influence is identified. Groundwater pressure does not affect advective transport or mixing *per se*, but gradients in groundwater pressure do. Therefore a local change in groundwater pressure can affect this process indirectly, via changes in the groundwater flow.

Gas phase flow

No direct influence is identified. Gas phase flow can affect advective transport and mixing indirectly, since its presence may affect the groundwater flow field (two phase bubble flow, see e.g. Nicklin 1962). Additionally, trapped gas can block pores and fractures, influencing groundwater flow.

Repository geometry

No direct influence is identified. The repository geometry influences the groundwater flow, and so influences advective transport and mixing indirectly.

Fracture and pore geometry

No direct influence is identified. The fracture and pore geometry define the hydraulic properties of the rock, and thus influence advective transport indirectly via groundwater flow.

Table 5-1. Direct influences of defined geosphere variables on the process "Advective transport/ mixing of dissolved species" and a short indication of how the influences are handled in the safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.2.7)
Temperature in bedrock	No, but indirectly via changes in groundwater flow: the temperature affects groundwater viscosity and density, which might induce density-driven groundwater flow and advection of solutes.	–	
Groundwater flow	Yes.	All	The magnitude and direction of groundwater flow is used as input to the solute transport model in the geosphere (Román-Ross et al. 2014). This input is obtained from hydrogeological modelling, see Section 3.2. See also Chapter 6 for the suggested handling in radionuclide transport.
Groundwater pressure	No, but indirectly via the influence of groundwater pressure gradients on groundwater flow, see Section 3.2.	–	
Gas phase flow	No, but indirectly through the influence of gas phase flow on groundwater flow, see Section 3.2.	–	
Repository geometry	No, but indirectly via groundwater flow, see Section 3.2.	–	
Fracture and pore geometry	No, but indirectly via groundwater flow, see Section 3.2.	–	
Rock stresses	No, but indirectly via groundwater flow, see Section 3.2.	–	
Matrix minerals	No direct influence. Indirectly via groundwater composition which is affected by interaction with matrix minerals. See further Section 5.5.	–	
Fracture minerals	No direct influence. Indirectly via groundwater composition which is affected by interaction with fracture minerals. See further Section 5.6.	–	
Groundwater composition	Yes.	All	Aqueous concentrations are included in solute transport calculations (Román-Ross et al. 2014). See also Chapter 6 for the suggested handling in radionuclide transport.
Gas composition	No, but indirectly via groundwater composition.	–	
Structural and stray materials	No, but indirectly via groundwater flow, and groundwater composition.	–	
Saturation	No, but indirectly via groundwater flow, Section 3.2.	–	

Rock stresses

No direct influence is identified. Rock stresses may affect advective transport indirectly via groundwater flow, since they may affect the porosity and fracture geometry of existing rock fractures, and initiate fracturing. These processes may create preferential paths for groundwater flow.

Matrix minerals

No direct influence is identified. Advection is influenced by matrix minerals indirectly, via groundwater composition which is affected by matrix diffusion and interaction with matrix minerals.

Fracture minerals

No direct influence is identified. Advection is influenced by fracture minerals indirectly, via groundwater composition which is affected by interaction with fracture minerals.

Groundwater composition

The magnitude of advective transport of a solute is proportional to its aqueous concentration, and so the groundwater composition is directly related to advective transport and mixing. Groundwater composition also has an indirect effect, via the influence of density-differences on groundwater flow, see Section 3.2.

Gas composition

No direct influence is identified. The gas composition is in equilibration with dissolved gas composition in the groundwater. Therefore, it has an indirect effect on advective transport and mixing via the groundwater composition.

Structural and stray materials

No direct influence is identified. Structural materials such as the grouting have an indirect effect on advective transport as they alter the groundwater flow, see Section 3.2. Structural materials may also affect local advective transport and mixing indirectly via changes to the groundwater composition resulting from dissolution and precipitation reactions.

Saturation

No direct influence is identified. Saturation has an indirect effect on advective transport and mixing via its influence on groundwater flow.

Explanation of Table 5-2

Temperature in bedrock

No direct influence is identified.

Groundwater flow

No direct influence is identified. Indirectly, advective transport of solutes may affect the density of the groundwater (groundwater composition) and thereby the density driven flow, see Section 3.2 (Groundwater flow).

Groundwater pressure

No direct influence is identified.

Gas phase flow

No direct influence is identified. Advective transport of solutes may influence the groundwater composition which may result in local gas generation or dissolution of gas.

Repository geometry

No direct influence is identified.

Fracture and pore geometry

No direct influence is identified. Advection and mixing can have an indirect effect on the fracture and pore geometry via groundwater composition: the transport of dissolved species into fractures and pores may lead to precipitation reactions or the dissolution of fracture minerals, which affects the geometry.

Table 5-2. Influences of the process “Advective transport/mixing of dissolved species” on defined geosphere variables, and a short indication of how this may be handled in safety assessment. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.2.7)
Temperature in bedrock	No direct influence.	–	
Groundwater flow	No direct influence. Indirectly, advective transport of solutes may affect the density of the groundwater (groundwater composition) and thereby the density driven flow, see Section 3.2 (Groundwater flow).	–	
Groundwater pressure	No direct influence.	–	
Gas phase flow	No direct influence. Indirectly, advective transport of solutes may result in local gas generation or dissolution of gas via its influence on groundwater composition. See Section 3.3 (Gas flow/dissolution).	–	
Repository geometry	No direct influence.	–	
Fracture and pore geometry	No, but indirectly via groundwater composition and dissolution/precipitation reactions.	–	
Rock stresses	No direct influence.	–	
Matrix minerals	No direct influence. Indirectly, advection induced changes in groundwater composition may result in matrix diffusion followed by dissolution/precipitation reactions. See further Section 5.5 (Reactions groundwater/matrix minerals).	–	
Fracture minerals	No, but indirectly via groundwater composition and dissolution/precipitation reactions. See further Section 5.6 (Dissolution/precipitation of fracture-filling minerals).	–	
Groundwater composition	Yes.	All	The evolution of the groundwater composition is modelled by stream-line simulations (Román-Ross et al. 2014; regarding estimated groundwater compositions from Auqué et al. 2013). The advective transport of radionuclides is handled by means of a mixed compartment model, see Chapter 6.
Gas composition	No, but indirectly via groundwater composition.	–	
Structural and stray materials	No, but indirectly via groundwater composition.	–	
Saturation	No direct influence. Indirectly, gas generation or gas dissolution may result from advection induced changes in groundwater composition. This may lead to local changes in the degree of saturation in parts of the rock volume.	–	

Matrix minerals

No direct influence is identified. Advection and mixing can have an indirect effect on the matrix minerals, via groundwater composition, matrix diffusion, and dissolution/precipitation reactions.

Fracture minerals

No direct influence is identified. Advective transport can have an indirect effect on the fracture minerals, via groundwater composition. The transport of dissolved species may lead to the precipitation of secondary minerals or the dissolution of existing fracture minerals.

Groundwater composition

The groundwater composition is directly influenced by advective transport and dispersive mixing of different constituents. The evolution of the groundwater composition is modelled by stream-line simulations (Román-Ross et al. 2014; regarding estimated groundwater compositions from Auqué 2013). The advective transport of radiounuclides is handled by means of a mixed compartment model, see Chapter 6.

Gas composition

No direct influence is identified. Advective transport and mixing affects the gas composition indirectly, via the groundwater composition. The advective transport of dissolved gases affects their aqueous concentration and thus the gas phase composition via Henry's law.

Structural and stray materials

No direct influence is identified. Advective transport and mixing can affect the structural and stray materials indirectly via the groundwater composition, as certain dissolved constituents can enhance the degradation of stray materials such as concrete and metal.

Saturation

No direct influence is identified. Advection induced changes in groundwater composition may promote gas generation or gas dissolution. This may lead to local changes in the degree of saturation in parts of the rock volume.

5.2.3 Boundary conditions

The boundary conditions for advection and dispersion processes are the groundwater flow field and the aqueous chemical composition in the biosphere, barriers and different parts of the geosphere. Changes in the climate and shoreline position will affect the composition of the water entering the geosphere, which in turn may lead to long-term changes in the groundwater composition.

5.2.4 Model studies/experimental studies

There are several modelling studies evaluating the role of advection and dispersion processes in typical Swedish granitic rocks. The Forsmark and Laxemar/Simpevarp sites have been modelled within the site investigation programme of SKB and in reports supporting the SR-Site application, using models incorporating e.g. density driven flow, diffusive exchange of salt between flowing water and water in the rock matrix, and advection–dispersion (see e.g. Joyce 2010a, b, Selroos and Follin 2010, SKB 2008d, Hjerne et al. 2010 and references therein). The advective solute transport models rely on, assumed or modelled water flow rates. Underlying hydrogeological modelling studies are further described in Section 3.2. Experimental studies that provide valuable information on advective solute transport in the Forsmark area include numerous cross-hole tracer tests performed within the SKB investigation programmes (Hjerne et al. 2010). A compilation and analyses of these tests with a focus on the relationship between the conservative tracer mean residence time and fracture hydraulic parameters is reported in Hjerne et al. (2010).

Further model and experimental studies are listed in the Geosphere process report for the safety assessment SR-Site (SKB 2010e) that highlight e.g. the importance of determining relevant effective porosities for use in estimations of travel times and the conceptual uncertainties (scale dependency) involved in estimations of dispersivity factors in modelling, in particular for fractured rock with high spatial variability. The physics of groundwater flow and solute transport in heterogeneous porous media and the derivation of mathematical representations of these processes on a macroscopic level are also rigorously described in e.g. Bear and Cheng (2010). Advective solute transport and dispersive mixing play important roles in the estimation of the long term evolution of the groundwater composition, and a list of studies addressing relevant aspects is also included in SKB (2010e). These include a number of model studies carried out in conjunction with field experimental studies in Sweden, e.g. 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, 2003, Poteri et al. 2002).

5.2.5 Natural analogues/observations in nature

Natural analogue sites and underground rock facilities demonstrate the existence and importance of advection and dispersion processes. Statistical multivariate analysis tools and general geochemical reaction path codes have been used to describe and distinguish the major effects of hydrochemical mixing conditions in the analogue studies at Oklo and Palmottu (Laaksoharju et al. 1999a, Gurban et al. 1998, 2003), at Äspö (Pitkänen et al. 1997, Laaksoharju et al. 1999b) and at several other Fennoscandian sites (Puigdomenech 2001, Pitkänen et al. 1998, 1999, 2004, Laaksoharju et al. 2008a, b, c, 2009). A more detailed description of these studies and their implications on the choice of handling within SR-Site is provided in SKB (2010e).

5.2.6 Time perspective

Advective solute transport in the geosphere is modelled over the entire time-span of relevance for the SR-PSU safety assessment (Román-Ross et al. 2014). The extent and direction of solute transport by advection will change in response to the prevailing groundwater flow field. Dynamic changes in hydraulic properties are expected, particularly as a consequence of periglacial permafrost and postglacial ice melting (see further Section 3.2).

5.2.7 Handling in the safety assessment

Advective transport by flowing groundwater is incorporated in the modelling of solute transport in all SFR compartments and in the geosphere. For radionuclide transport modelling in the geosphere a coarsely discretised mixed compartment model approach is used (see further Section 6.2). The advective transport of groundwater constituents (excluding radionuclides) is handled within SR-PSU through stream-line one dimensional modelling (Román-Ross et al. 2014).

Handling relative to time periods, climate domains, and events

Advective transport and dispersion is related to the prevailing flow field, flow rates and aqueous solute concentrations (e.g Auqué et al. 2013) which are regarded as boundary conditions. The processes of advection and dispersion are therefore handled in conjunction with the water transport and aqueous speciation in relation to different time periods, climate domains and events. The handling of groundwater flow and radionuclide transport is discussed in Sections 3.2 and 6.2 respectively.

Excavation/operation/re-saturation period

Advective transport of solutes is directed along the main water flow direction from the geosphere into the repository volume (recharge), and very limited, or no release of dissolved components from the SFR repository into the geosphere is expected. This is considered as the initial state or starting point of the safety assessment (**Initial state report**).

Periods of the temperate climate domain

Advective solute transport in the geosphere is modelled throughout the temperate period (Román-Ross et al. 2014) and the prevailing groundwater composition (ranges of solute concentrations) is used as input for the given period (Auqué et al. 2013).

Periods of the periglacial climate domain

Advective solute transport is limited since the flow is expected to be restricted under frozen conditions. Prevailing groundwater composition is modelled (Román-Ross et al. 2014).

Periods of the glacial climate domain

Advective solute transport is related to the prevailing water flow field during the time period. It is however not included in modelling of the processes. A safety assessment scenario, in which there is no retention in the geosphere is however included in SR-PSU.

Earthquakes

The consequences of an earthquake breaching the barriers of the Silo are assessed within defined artificial "earthquake" loads for different repository failure scenarios, and where no saturation of the system was assumed as a pessimistic assumption (Georgiev 2013). Increased advective transport as a result of pressure waves creating short temporal groundwater movements is expected in the geosphere but not considered as an essential aspect of this assessment. However the radiological consequences of such an event are handled in a pessimistic residual scenario in radionuclide transport modelling (**Radionuclide transport report**).

Handling relative to geosphere variables

The extent and direction of advective transport of solutes is proportional to the water flow field and flow rates as well as the local dissolved solute concentrations. The groundwater flow and solute concentrations are incorporated as boundary conditions in the advective transport calculations in the safety assessment.

5.2.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Advection and dispersion processes can be considered mature science and the conceptual uncertainties are small.

Model simplification uncertainties

The one dimensional stream-line approach for modelling groundwater solute transport in the geosphere (Román-Ross et al. 2014) neglects hydrodynamic dispersion and mixing between flow paths.

5.2.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in the SR-PSU. All references have undergone a documented factual- and quality review by SKB or have been published by refereed scientific journals.

5.3 Diffusive transport in the rock mass

5.3.1 Overview/general description

This text concerns liquid phase diffusive transport of solutes in the stagnant pore water of the rock matrix, as well as in stagnant fracture water[5]. Such transport is of consequence both for the evolution of geochemical conditions of the repository host rock, as well as for the retardation of radionuclides escaping from the repository. Diffusive transport is also of importance in flowing water, with respect to mixing. However, such aspects are omitted from this present section, as mixing is described in Section 5.2.

The description of the process and supporting observations should be more or less independent of the specifics of the repository, as long as it is situated in crystalline rock. Therefore, part of this text is reproduced from the corresponding section of the SR-Site Geosphere process report (SKB 2010e, Section 5.3). However, where warranted the text is modified to better represent the SFR repository.

Diffusion in the rock matrix

Liquid phase diffusion, as described in this section, takes on importance where advective transport with flowing water is small. Such conditions prevail in the micropores of the rock matrix, where the water flow is insignificant. Solutes transported in discrete fractures by flowing water may enter these micropores through diffusion, a phenomenon known as matrix diffusion (e.g. Neretnieks 1980).

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[5] Solid phase diffusion is not addressed.

Matrix diffusion is a very important retention mechanism in the geosphere, both for sorbing and non-sorbing radionuclides, see Section 6.2, as well as for other species in tracer amounts. Matrix diffusion also evens out concentration differences of major groundwater constituents along flow paths. This is of importance for the groundwater salinity, as an example. In case of intruding waters of elevated solute concentrations, the micropores of the rock matrix function as a sink whereto the surplus of solutes can diffuse. Conversely, in the case of an intrusion of dilute water, the micropores function as a source of solutes. Matrix diffusion also plays an important role in the long-term evolution of hydrogeochemical conditions of the repository host rock, by way of bringing reactants in the fracture water into the rock matrix where reaction can occur. This is especially of importance for the redox conditions at SFR. For example, dissolved oxygen that infiltrates the host rock in hydraulically conductive fractures will diffuse into the rock matrix where reaction can occur. Consequently, matrix diffusion aids in the buffering against changes in redox conditions (e.g. Sidborn et al. 2010).

For sorbing species, matrix diffusion gives access to the very large inner surfaces of the rock matrix where sorption can occur. These surfaces can typically be three to six orders of magnitude larger in area than the surfaces of the fractures where advective transport occurs. For example, measurements of the surface area for major rock types at the Forsmark site by the BET (Brunauer Emmet Teller) technique (Byegård et al. 2008) suggest internal surface areas on the order of 10^4–10^5 m^2/m^3. This should be compared to the flow-wetted fracture surface area per unit volume of rock suggested in SKB (2010b, Table 6-78), which is 0.6 m^2/m^3 for rock down to an elevation of –200 m.

For non-sorbing species, which are not retarded by interactions with fracture mineral surfaces, the access to stagnant pore water will to some extent retard the solutes, compared to the flowing water. For example, if a pulse release of non-sorbing radionuclides occurs from the engineered system, matrix diffusion may lower the released peak activity to the biosphere, see details in Section 6.2. The same applies in case a pulse of groundwater of different composition intrudes the repository host rock.

An on-going release of radionuclides is expected from SFR, particularly following the loss of barrier function in the Silo and BMA. However, the release rates and release flow paths will vary. On-going release reduces the diffusive gradients into the pores of the matrix, especially in the case of non-sorbing nuclides, and this lessens the effect of matrix diffusion on the maximum radionuclide concentrations reaching the biosphere, see further discussion in Section 6.2.

The key entities needed when assessing the diffusive properties of the rock matrix are the effective diffusivity D_e (m^2/s) and the storage capacity α (–) for the species in the rock matrix, and the connectivity of the porous system. The storage capacity of the rock matrix ($\alpha = \varepsilon + K_d\rho$) is the combined storage capacity available for solutes in the pore water and species sorbed on mineral surfaces. It is common to use the apparent diffusivity D_a (m^2/s) when modelling matrix diffusion:

$$D_a = \frac{D_e}{\varepsilon + K_d \rho} \qquad \text{Equation 5-1}$$

where ε (–) is the connected porosity, K_d (m^3/kg) the sorption partitioning coefficient, and ρ (kg/m^3) the rock density. For non-charged species that do not interact with the rock matrix, the effective diffusivity can be obtained from the product of the diffusivity of the species in free solution D_w (m^2/s) and the formation factor[6] F_f (–) (Neretnieks 1980). A prerequisite for this is that the characteristic length of the pores is much larger than the size of the solutes, otherwise size-exclusion effects may occur. For charged species, the diffusion may be decreased by ion exclusion or enhanced by surface diffusion, which is conceptualised as an enhanced diffusion rate in the electrical double layer at the mineral surface, due to an increased cation concentration gradient (e.g. Olin et al. 1997, Ohlsson 2000, Axe et al. 2002). The key entity for storage of non-sorbing solutes in the pore water is the connected porosity ε (–). Matrix diffusion may occur in all types of connected porosity, including grain boundary pores; micro fractures; sheet silicate pores; and ruptured fluid inclusions (Möri et al. 2003a, Ota et al. 2003).

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[6] It should be noted that the formation factor in some instances in SR-Site is denoted F_m.

Although there is a consensus among experts that matrix diffusion occurs in nature, there have been different opinions as to the depth to which diffusion can reliably be assumed to penetrate the crystalline rock matrix. An entity crucial for the penetration depth is the pore connectivity. In SR-Site it was suggested that the pore connectivity of crystalline rock representative for the Forsmark site is, at least, on the decametre scale (SKB 2010b, e). This was supported by arguments in Möri et al. (2003a), Löfgren and Neretnieks (2006), Crawford (2008) and Waber et al. (2009a, b). It is also the current position of SKB that the microporous system of the SFR host rock is connected on all scales relevant for the safety assessment.

Mineral surfaces of crystalline rock, such as granite, are most often negatively charged under natural groundwater conditions; thus there is a repulsion of negatively charged ions close to the surfaces (Stumm and Morgan 1996). For very small pores, this means that anions are excluded from an important fraction of the pore space, resulting in a smaller effective cross section area for diffusion and lower diffusion rates. Since matrix diffusion is the most important retention mechanism for anions, anion exclusion would promote transport of anions such as I-129 by advection in the water-conducting fractures through the geosphere. In SR-Site it was suggested that the anion exclusion reduction factor is, on average, half an order of magnitude (SKB 2010b, Section 6.8). This can be compared with the assumption of the Finnish programme, where the reduction factor has been suggested to be one order of magnitude (e.g. Valkiainen et al. 1996, Olin et al. 1997).

Surface diffusion has been proposed as a process explaining observations of increased diffusion rates for some cations in crystalline rock (e.g. Ohlsson and Neretnieks 1998). This means that sorbed cations in the electrical double layer, both in the Stern layer and in the diffuse layer, may be affected by increased concentration gradients and thus be transported along the solid surfaces in a diffusion-like process. The phenomenon is well known in science and has been argued to be important for diffusion in bentonite buffers. However, its effectiveness in crystalline rock has not been commonly accepted. Thus, surface diffusion is usually neglected in safety assessments, which is regarded as a pessimistic approach (at least from the perspective of radionuclide transport, see discussion in Section 6.2), since an increased diffusivity in the rock matrix would increase the retention in the geosphere.

The stability of the matrix pore system over longer time periods is a crucial and difficult question. It has been shown that when applying pressure to a de-stressed rock sample in the laboratory, the porosity decreases (e.g. Jacobsson 2007) and so does the effective diffusivity (e.g. Skagius and Neretnieks 1986). It is conceivable that the porosity will be slightly compressed in situ as a result of the ice load during glacial periods. The magnitude and importance of such potential compression remain to be investigated.

Alterations in the flow field due to geological and climatic changes may affect the flow paths and thus also the contact area (flow-wetted surface) between flowing water and the rock matrix. This will in turn affect the retention capacity due to matrix diffusion. This may be of importance for a repository such a SFR, where the radionuclide release is ongoing upon saturation, although at a low and non-uniform rate. As the flow paths change, the radionuclides will come into contact with new rock volumes and thus gain access to microporous systems that have not previously been exposed to radionuclides, see also discussion in Section 6.2.

Precipitation and dissolution of mineral phases maybe caused by changes in water composition from natural causes or by materials introduced in the repository. Changes in mineral phases, due to precipitation, dissolution, weathering, oxidation, and other alteration processes, may affect the available connected porosity of the rock matrix (e.g. Kuva et al. 2012). Under natural circumstances the above mentioned processes are so slow that their effect during the assessment time frame is very limited. However, an issue that deserves investigating is whether an alkaline pH plume, originating from groundwater in contact with cementations materials in the repository, may affect rock mineral phases in the repository discharge areas (see also Section 5.4). As result of this plume, part of the microporous system may be clogged, which could, at least locally, hinder matrix diffusion.

The discussion given in this section, as well as the modelling in SR-Site and SR-PSU, is based on Fickian diffusion theory, even though it could be argued that the Maxwell–Stefan diffusion theory better handles multi-component mass transfer (Krishna and Wesselingh 1997), especially in an electrically charged rock matrix. However, as the concentrations of radionuclides are expected to be very low in the geosphere, it is judged that a multi-component mass transfer approach is generally not needed. Where there are sudden and major changes in the water composition, and thus extensive migration of groundwater constituents in the pore water, Fickian diffusion theory may be inadequate. However, even if it is conceivable that the groundwater composition may undergo major changes, also at repository depth, such changes will not be sudden, but take place over years to millennia. In short-term tracer tests, multi-component mass transfer effects cannot be ruled out, which should be kept in mind when evaluating the data.

Diffusion in stagnant fracture water

Substantial areas within individual water-conducting fractures may contain effectively stagnant water. It has been suggested that if these zones are sufficiently large and accessible by diffusion from flow channels of limited width, the overall retardation effect may be some orders of magnitude greater than that predicted in their absence (Crawford and Sidborn 2009). The retention capacity of the effectively stagnant fracture water is generally limited, although further diffusion from these regions into the rock matrix can provide much additional retention over longer timescales. The same arguments can be made for fractures containing a mix of flow paths, stagnant water, and relatively porous fracture infillings. Solutes may diffuse from the flow path into such fracture infillings and further on into the rock matrix. Diffusion into effectively stagnant zones (which in a tracer test might be reasonably expected to include non-equilibrium diffusion between fast and slow moving flow streamlines) has been used to explain pronounced tailing in the breakthrough of short-term in situ tracer tests that could not be explained by diffusion into the rock matrix alone (e.g. RETROCK 2004, Neretnieks 2007).

Diffusion may also occur into stagnant water of fractures intersecting the flow path. Based on data from the Forsmark and Laxemar site investigations, it may be suggested that the diffusion capacity into intersecting fractures, where no flow can be detected, would be on the same order of magnitude as diffusion into the rock matrix. This is also discussed in Löfgren (2014), based on measurements at the SFR site. Due to the relatively large apertures of the fractures, compared to the apertures of micropores in the rock matrix, exclusion effects such as size exclusion and anion exclusion can likely be disregarded. This may be of interest when modelling the transport of colloids from the repository to the surface system, as colloids are generally said to be excluded from the micropores. These issues need to be evaluated further in conjunction with flow calculations to assess their importance at the site.

5.3.2 Dependencies between process and geosphere variables

This section outlines the dependences between the process "diffusive transport in the rock mass" and defined geosphere variables that are commonly expected in fractured crystalline rock. This means that these dependences are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-3 outlines how the process is influenced by the defined geosphere variables, while Table 5-4 outlines how this process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event the described influence is relevant. The influence between the process and each geosphere variable is elaborated upon below.In the rightmost column there is a brief description of the handling of the influence in the safety assessment SR-PSU. In Section 5.3.7, this handling is discussed.

Explanation of Table 5-3

Temperature in bedrock

The temperature affects the diffusivity of the solutes. To a minor extent the temperature may also affect the pore space geometry as result of thermal expansion of mineral grains, thereby indirectly affecting the process. However, this latter effect should be overshadowed by other natural variability.

Groundwater flow

The solute exchange between flowing fracture water and stagnant water in the fractures and rock matrix is affected by the groundwater composition. The groundwater composition is in turn affected by the groundwater flow, as solutes can be transported to or away from the flow path/stagnant water interface.

Table 5-3. Direct influences of defined geosphere variables on the process "diffusive transport in the rock mass" and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.3.7)
Temperature in bedrock	Yes.	All	Handled as input data uncertainty in modelling.
Groundwater flow	No, but indirectly through: Groundwater composition.	All	–
Groundwater pressure	No.	All	–
Gas phase flow	No, but indirectly through: Groundwater composition.	All	–
Repository geometry	No.	All	–
Fracture and pore geometry	Yes.	All	Fracture and pore geometries are essential for this process. Site specific data are used.
Rock stresses	No, but indirectly through: Fracture and pore geometry.	All	Handled as input data uncertainty in modelling.
Matrix minerals	Yes. Mineral surfaces attract or repulse diffusing solutes.	All	Handled by assigning an anion exclusion factor for anions, and by incorporating K_d data in the apparent diffusivity for sorbing species.
Fracture minerals	Yes.	All	The potential influence of fracture minerals on diffusion is typically neglected.
Groundwater composition	Yes.	All	The effect of groundwater composition on diffusivity is handled as input data uncertainty. Solute concentration gradients are accounted for in modelling, as the driving force for matrix diffusion.
Gas composition	No, but indirectly through: Groundwater composition.	All	–
Structural and stray materials	No, but Indirectly through: Groundwater composition.	All	–
Saturation	Yes.	E/O/S	No modelling including matrix diffusion is performed during this period for the geosphere.
		T/P/G/EQ	Fully saturated host rock assumed.

Groundwater pressure

In an incompressible medium such as water, the groundwater pressure has no practical implications for the diffusivity.

Gas phase flow

Gases may dissolve and affect the groundwater composition and thereby indirectly affect the diffusion. In the case of a gas phase flow, giving rise to a partly unsaturated fracture system, this would affect the contact area between flowing and stagnant water volumes. However, such gas flows from the SFR repository are not expected to be sustained (see Section 3.3).

Repository geometry

Diffusion, which should be considered as a small-scale process, is not directly affected by the repository geometry.

Fracture and pore geometry

Liquid phase diffusion occurs in the water filled voids of the rock, i.e. the fracture system and the microporous network of the rock matrix. Accordingly, as also discussed in Section 5.3.1, their geometries are essential.

In addition, the contact area between flow paths and stagnant water volumes is essential for assessing the influence of diffusion on the water composition.

Rock stresses

Changes in the rock stress, due to for example the formation and melting of an ice sheet during the glacial period, will affect the fracture and pore geometry. Thereby the effective diffusivity will be indirectly affected. This effect is estimated to be moderate (SKB 2010b, Section 6.8).

Matrix minerals

The electric charge of the matrix mineral surfaces affects the diffusion by way of anion exclusion and possibly surface diffusion (see Section 5.3.1). Also, importantly, it affects how strongly different solutes will sorb to the mineral surfaces, which in turn affects how far they will penetrate into the rock matrix during a given time.

Fracture minerals

If fracture minerals have a very low effective diffusivity, they can block the transport paths into the rock matrix. However, this is not generally expected at the Forsmark site (Byegård et al. 2008). If the solutes sorb much more strongly to the fracture minerals than to the matrix minerals this could be seen as an effective way of (partly) hindering the solutes from entering the rock matrix.

Groundwater composition

The groundwater composition is essential for diffusion. If considering the diffusion of an element, its speciation largely determines the diffusivity in free solution D_w. Also, the speciation determines to what extent there will be interactions with the matrix minerals, and whether the species are subjected to anion exclusion, surface diffusion, and sorption. Furthermore, the groundwater composition affects the properties (e.g. viscosity) of the fluid surrounding the diffusing solutes, thus affecting the diffusivity.

The concentration gradient is the driving force for diffusion (if assuming Fickian diffusion) wherefore composition differences between the flowing and stagnant water are essential when assessing the diffusion rate.

Gas composition

Gasses may dissolve and affect the groundwater composition and thereby indirectly affect the diffusion.

Structural and stray materials

Structural and stray materials such as rock reinforcement and grouting may affect pH, redox conditions, colloid concentration, etc., of the groundwater. This may in turn affect the speciation and concentrations of other solutes in the groundwater. It is conceivable that a strongly affected groundwater (e.g. an increased pH) may lead to precipitation at the fracture surface and even (in extreme cases) affect the microporous system by way of clogging. For the SFR repository, the same materials are abundant within the rock vaults and the direct effect of structural and stray materials on the groundwater composition is accordingly dwarfed.

Saturation

The water filled pore space geometry, facilitating liquid phase diffusion, is affected by the degree of saturation. In the case of gas filled fractures or pores, diffusion in the gas phase may be of importance. However, such gas filled voids are not expected to be sustained at depth in the SFR host rock (see Section 3.3). The exception may be adjacent to the rock caverns during the excavation, operation, and saturation period, or in very shallow rock such as outcrops.

Table 5-4. Direct influences of the process "diffusive transport in the rock mass" on the defined geosphere variables, and a brief description of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.3.7)
Temperature in bedrock	No.	All	–
Groundwater flow	No, but indirectly through: Groundwater composition.	All	Density driven flow is not considered in SR-PSU. Accordingly the effects of diffusion in the rock mass on groundwater flow are disregarded.
Groundwater pressure	No.	All	–
Gas phase flow	No, but indirectly through: Groundwater composition.	All	–
Repository geometry	No.	All	–
Fracture and pore geometry	No, but indirectly through groundwater composition and precipitation and dissolution.	All	See processes Reactions groundwater / rock matrix (Section 5.5) and Dissolution/precipitation of fracture-filling minerals (Section 5.6).
Rock stresses	No.	All	
Matrix minerals	No, but indirectly through groundwater composition and precipitation and dissolution.	All	See processes Reactions groundwater / rock matrix (Section 5.5).
Fracture minerals	No, but indirectly through groundwater composition and precipitation and dissolution.	All	See processes Dissolution/precipitation of fracture-filling minerals (Section 5.6).
Groundwater composition	Yes. Diffusion redistributes solutes.	All	Diffusional solute exchange between flow paths and stagnant water volumes is accounted for in modelling groundwater composition.
Gas composition	No, but indirectly through: Groundwater composition.	All	–
Structural and stray materials	Yes. Diffusion may aid degradation.	All	The integrity of structural and stray materials is not a focus of attention in SR-PSU. This is handled through design of the support of the tunnel walls (**Barrier process report**).
Saturation	No.	All	–

Explanation of Table 5-4

Temperature in bedrock

The temperature in the bedrock is not dependent on diffusion of solutes.

Groundwater flow

Groundwaters of different compositions have different densities. This may give rise to density driven flow, providing there are large enough salinity differences. As diffusional solute exchange between the flowing and stagnant water affects the groundwater composition (including the salinity), the process may indirectly affect the groundwater flow. However, this is thought to be of minor importance for the SFR host rock (see Section 3.2).

Groundwater pressure

The groundwater pressure is not directly dependent on diffusion.

Gas phase flow

Diffusion affects the groundwater composition and may therefore indirectly affect the gas phase flow, if solutes come out of solution or gas is dissolved.

Repository geometry

Diffusion does not directly affect the repository geometry.

Fracture and pore geometry

Solutes diffusing into stagnant water volumes may to a minor extent give rise to mineral precipitation, alteration, and dissolution, which may change the fracture and pore geometry. It is conceivable that the cementitious materials in the repository will give rise to an alkaline pH plume in the discharge area. This plume may also have elevated concentrations of solutes originating from the degradation of the cementitious materials. These conditions may affect the flow path and the rock surrounding the flow path (e.g. Smellie 1998). Especially the potential for precipitation in the rock matrix may be of concern for SFR, if it leads to (partial) clogging of the microporous system. In addition, the alteration of primary matrix minerals (e.g. quartz) to secondary mineral phases of larger specific volume may affect the micropore geometry (Sidborn et al. 2014). Precipitation may also alter the fracture geometry available for flow and diffusive exchange.

Rock stresses

The rock stresses are independent of diffusion.

Matrix minerals

Matrix diffusion affects the pore water composition, which affects alteration, dissolution, and precipitation reactions of matrix minerals. Diffusion aids in transporting reactants and reaction products to and from the mineral surfaces. The pore water composition may also affect the tendency of solutes to sorb on mineral surfaces (see Section 5.4).

Fracture minerals

Fracture minerals are affected by the contacting water composition through precipitation and dissolution. The groundwater/pore water composition is in turn affected by diffusion. Accordingly diffusion affects fracture minerals by way of promoting alteration, precipitation, and dissolution.

Groundwater composition

Diffusional exchange between flowing and stagnant water volumes greatly affects the composition of both groundwater and pore water. It should be kept in mind that the great majority of the water existing at depth is stagnant.

Gas composition

Liquid phase diffusion affects the groundwater composition and may therefore indirectly affect the gas composition, in case solutes come out of solution or gas is dissolved.

Structural and stray materials

Diffusion in cementitious materials may aid degradation, by way of transport of reactants and reaction products. If diffusion brings corrodants to metallic components such as rock reinforcements, the process is of consequence for the integrity of the component.

Saturation

The degree of saturation is independent of liquid phase diffusion.

5.3.3 Boundary conditions

For the process of diffusion in the rock matrix, and in stagnant fracture water volumes, boundary conditions at the geosphere/biosphere and geosphere/engineered system interfaces have only indirect consequences. The most important indirect consequence is that solutes are transported over these boundaries, affecting the groundwater composition along flow paths, which in turn affects local concentration gradients of importance for the diffusion rate.

Local boundary conditions include the contact area between flow paths and stagnant water volumes, together with concentration gradients. According to the Maxwell–Stefan theory, differences in chemical potential, as opposed to difference in concentration, constitute the driving force for migration. In this respect it may be appropriate to mention that local electrical potential gradients (earth currents) in the rock matrix may affect ionic solutes in an analogue way to diffusion (see Section 5.12).

Very small-scale boundary conditions for matrix diffusion concern the properties, especially the electric charge, of the mineral surfaces surrounding the micropores and fractures. This affects not only sorption (see Section 5.4) but also anion exclusion and surface diffusion.

Finally, a necessary condition for liquid phase diffusion is the existence of water. This condition is always fulfilled at depth during the temperate climate domain. However, in very shallow rock such as outcrops, part of the rock may have dried out. This results in gas filled fractures and pores, prohibiting liquid phase diffusion. Another prerequisite is that the water is in liquid form. This means that the process is halted if the water freezes, as may be the case during periods of the periglacial and glacial climate domains. It is uncertain to what extent the micropore water freezes, even under conditions where the fracture water is frozen (cf. Section 5.11).

5.3.4 Model studies/experimental studies

Matrix diffusion in rock is a process that has been studied for decades (e.g. Garrels et al. 1949, Neretnieks 1980). It is one of the processes that were addressed in the RETROCK project, aimed at examining how the retention and transport of radionuclides should be represented in safety assessment models for deep geological repositories in fractured rock (RETROCK 2004, 2005). Matrix diffusion has been further studied by SKB as part of the site investigations and site descriptions at Forsmark and Laxemar, for the KBS-3 repository. In addition there are recent studies supporting (part of) this process description (e.g. Löfgren et al. 2009, Nilsson K et al. 2010, Löfgren 2014).

The existence of an interconnected system of microfractures and micropores in granitic rock, where matrix diffusion may occur, has been verified by experiments both in the laboratory and in the field. A compilation of such studies is given in Liu et al. (2006). Furthermore, a compilation of the SKB field work on tracer tests from 1977–2007 is given in Löfgren et al. (2007). Recent evidence from the LTDE-SD tracer test at the Äspö Hard Rock Laboratory verifies the existence of an interconnected microporosity on the decimetre scale (Nilsson K et al. 2010). Furthermore, evidence of large-scale pore connectivity comes from studies of the pore water salinity of the intact rock matrix, which suggests that the porous system is connected on at least the decametre scale (Waber et al. 2009a, b). Some examples of studies of matrix diffusion are outlined below.

Laboratory experiments with the purpose of determining diffusion data in the matrix of crystalline rock have been reported by many researchers in countries such as Sweden, Finland, the UK, Japan, Canada, Czech Republic, and Switzerland. Tracers penetrating through crystalline rock samples up to 12 cm in length have been observed (Löfgren and Neretnieks 2006). Many of these experiments have been performed on unaltered[7] rock, while very few have been performed on rock adjacent to fractures, fracture coatings or fracture filling material. Studies indicate that the porous media in or adjacent to fractures generally have higher porosities and diffusivities than the undisturbed rock (e.g. Byegård et al. 2002, 2008, Möri et al. 2003a, Widestrand et al. 2007, Kuva et al. 2012). Results from re-stressed rock samples in the laboratory indicate that the effective diffusivity is lower in samples under stressed conditions (Bradbury and Green 1986, Skagius 1986, Skagius and Neretnieks 1986).

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[7] In this sense we do not mean metamorphic alteration but chemical alteration due to adjacent flow paths at ambient or elevated (hydrothermal) temperatures.

Field-scale tracer tests have been performed at a number of sites around the world. However, in most cases these have been carried out in flowing water, focusing on obtaining breakthrough curves and from inverse modelling extracting information on matrix diffusion (see overview in Zhou et al. 2007). Only in a few cases, overcoring has been performed and direct evidence for matrix diffusion in the in situ rock matrix has been obtained. At 360 m depth in the Stripa mine in Sweden, such overcoring was performed and the tracer test resulted in diffusion profiles extending at least 40 cm into the undisturbed rock matrix (Birgersson and Neretnieks 1988, 1990). The results also indicate large variability in the diffusivities evaluated from the experiments, in spite of a (seemingly) relatively homogeneous rock matrix. Tracers penetrating the in situ rock matrix beyond a few centimetres have also been observed at the Canadian Underground Research Laboratory (Vilks et al. 2003). Similar observations have been made at the Grimsel Test Site in Switzerland (e.g. Möri et al. 2003b). Recently, tracer penetration up to 7 cm has been observed in the Äspö Hard Rock Laboratory within the LTDE-SD programme (Nilsson K et al. 2010). What is interesting to note from the penetration profiles is that they were poorly reproduced by modelling using a Fickian diffusion approach in homogenous media, and that heterogeneous diffusion was indicated (Nilsson K et al. 2010). These few in situ in-diffusion tracer tests, and others, show results that roughly support the conceptual understanding of diffusion of solutes in the rock matrix, although it appears that heterogeneous diffusion takes on an important role, at least on the scale of the experiments.

Based on the analogy between diffusion and electromigration, as described by the Einstein relation, formation factors have been estimated from measurements of the rock resistivity and estimates of the pore water electrical conductivity (e.g. Skagius and Neretnieks 1986, Löfgren and Neretnieks 2003, 2006, Crawford and Sidborn 2009, SKB 2010b). Loggings of many boreholes have been conducted within the site investigation programme for the KBS-3 repository, both in the laboratory on drillcore samples (e.g. Thunehed 2007) and in situ (e.g. Löfgren 2007). In situ loggings have also been performed in boreholes at the SFR site (Löfgren 2014). The in situ results indicate that the unaltered rock has a micropore connectivity on at least the metre-scale. However, in these in situ loggings an alternating electric current is used, which brings uncertainty to the validity of the observations regadring micropore connectivity. In addition, open fractures with stagnant water, and possibly also alteration zones around fractures, are found to increase the potential for migration. By comparing results from in situ and the laboratory, there are indications that the drillcore samples brought to the laboratory are stress-released and/or mechanically damaged, and might not be representative of in situ conditions (e.g. SKB 2010b, Section 6.8). See also Waber et al. (2009b) for an evaluation of perturbations on sample integrity by drilling and stress release.

The significance of anion exclusion has been studied by SKB on drill core samples from the Forsmark site in the laboratory (Löfgren et al. 2009). The effect of anion exclusion was found to be limited, at least at de-stressed conditions in the laboratory. However, the comparison of diffusive properties for anions and non-charged species was complicated by the fact that the tracer tests used different driving forces. Anion exclusion has also been studied in the LTDE-SD campaign, both in the laboratory (Vilks et al. 2005) and in situ (Nilsson K et al. 2010). In the laboratory part, through diffusion tracer tests on 16 drill core samples were performed. In these tests, the non-charged tracer HTO and the anionic tracer iodide simultaneously diffused through the rock samples. The results indicate that the anionic tracer, on average, had a half an order of magnitude lower effective diffusivity than the non-charged tracer. In these measurements, the ionic strength of the background solution was set to fairly well match that of the in situ groundwater. In the in situ part of LTDE-SD, penetration profiles for ^{22}Na and ^{36}Cl were compared and modelling suggests that the anion exclusion reduction factor is between half an order and one order of magnitude. Here it should be noted that the modelling failed to reproduce the general shape of the penetration profiles. Accordingly, numerical data should be used with care.

What can be suggested from measurements on Finnish crystalline rock is that the effect of anion exclusion is significant and reduces the effective diffusivity of anions by about one order of magnitude (Valkiainen et al. 1996, Olin et al. 1997). According to the electric double layer theory (e.g. according to Stumm and Morgan 1996), the thickness of the electrical double layer is greater at pore waters of low ionic strength. Based on this, one can assume that the effect of anion diffusion increases with decreasing pore water salinity, if the pore throats are very narrow. In practice, however, it has been observed on Finnish granite that the influence of the pore water ionic strength on anion exclusion is weak (Olin et al. 1997).

5.3.5 Natural analogues/observations in nature

Natural analogues in the form of geological formations with elevated natural radioactivity (and even sites with normal background radioactivity) can be used to verify matrix diffusion as a process that took place over long time spans, compatible with the expected timescale of relevance for a repository. Analogues of this type, found for example at Kråkemåla in Sweden, Palmottu in Finland, Alligator Rivers in Australia and Cigar Lake in Canada, offer an opportunity to achieve better process understanding (Miller et al. 1994, 2000). Measurements of concentration profiles in one fracture exposed in the Äspö tunnel and in a drillcore drilled from the surface have documented matrix diffusion of U and Cs on scales of some centimetres (Landström et al. 2001).

Concentration profiles from earlier uranium-series disequilibrium studies have been compared with model simulations (Rasilainen 1997) showing that it is possible to get an idea of the effects of matrix diffusion. Agreement between measured and simulated profiles indicates that the matrix diffusion models used are realistic. Since the applied models include sorption processes, it can be claimed that the analogue studies also verify the fact that combined matrix diffusion and sorption are active processes in situ. The occurrence of an altered zone with higher porosity and larger volumes of secondary minerals may enhance matrix diffusion (Smellie et al. 1986, Landström et al. 2001, Andersson et al. 2002a, Widestrand et al. 2007, Kuva et al. 2012).

A common natural analogue is oxidation fronts in the crystalline rock matrix at hydraulically conducting fractures, where oxidising meteoric water from the surface infiltrates the reducing interior of the bedrock. Oxidising agents thereafter penetrate the rock matrix by diffusion resulting in an oxidation front that may occur many decimetres from the fracture surface (RETROCK 2004).

Within the site investigation programme for the KBS-3 repository, the concentration of solutes of the freely flowing groundwater, as well as of the pore water of the rock matrix, has been measured. Evaluations of the data (e.g. Laaksoharju et al. 2008b, 2009, Waber et al. 2009a, b) have provided concentration profiles of the major groundwater constituents that in general are predictable. Outliers that, without closer examination, may indicate rock volumes with a non-connected microporous system are rare, if at all existing. In Laaksoharju et al. (2008b) and Waber et al. (2009b) it is proposed that the pore water of the target volume for the KBS-3 repository, that is the rock hosting the repository at depth at the Forsmark site, is saturated with water infiltrating the rock before the latest glacial period. This proposal is substantiated with isotope considerations. However, considering the scarcity of hydraulically conductive fractures in the rock volume, this means that solutes observed in the pore water characterisations would have had to diffuse many metres, sometimes tens of metres, through the rock volume from the nearest flowing fracture. In Waber et al. (2009a, b) matrix diffusion was identified to occur over several decametres into the rock matrix, as shown by the quantitative description of Cl^-, $\delta^{18}O$ and δ^2H profiles in the pore water.

Concentration data for the major constituent chloride (and also considering $\delta^{18}O$), in pore water studies at Laxemar (Laaksoharju et al. 2009, Waber et al. 2009a) may suggest that the freely flowing groundwater is fairly well equilibrated with the pore water in locations at shallow levels down to about 350 m depth. Inadequate data from Forsmark (Laaksoharju et al. 2008b, Waber et al. 2009b) precludes a quantitative interpretation, but transient conditions are likely in the upper 150 m. In contrast to the Laxemar situation, similar data from the Finnish site Olkiluoto indicate that the pore water and groundwater is not equilibrated at a depth of 420 m (Posiva 2009, Section 7.3.4). Anion exclusion is offered as one explanation for this (Posiva 2012, Section 3.1).

Concerning the effect of a hyperalkaline porewater on the microporous system wherein matrix diffusion occurs, this was a focus of attention in the Marqarin analogue study. The following conclusion was provided, directly relating to the impact on safety assessment (Smellie 1998, Section 12.3.4):

"The mineralogical alteration of wallrocks adjacent to fractures at Maqarin gives evidence that, initially, at least, the rock matrix is accessible to diffusion. Evidence from ^{226}Ra profiles in the rocks adjacent to fractures suggests that the matrix continues to be accessible to fluids from fractures. This important observation implies that matrix diffusion could continue to act as a retardation mechanism in the altered rock."

5.3.6 Time perspective

Diffusion is a relatively slow process. It is primarily the combination of matrix diffusion and sorption that gives the geosphere its retarding capacity for radionuclides and other solutes, as discussed in Section 6.2 Even with advective travel times of a few years, from the repository to the biosphere, sorbing solutes may be retarded by several orders of magnitude relative to this. On the other hand, for non-sorbing or very weakly sorbing solutes (e.g. ^{14}C) the effect of retardation is more pronounced on the peak release rates, in case of a pulse release, than on the arrival times (SKB 2010f). In case of ongoing release of non-sorbing species along the same flow path, the retardation effect of matrix diffusion decreases with the release time. Accordingly, in such a case diffusion into stagnant water volumes is of less importance for a safety assessment.

Liquid phase diffusion in stagnant water continues to be of importance for radionuclide retardation and groundwater composition throughout repository evolution and in every applicable event, as long as the water is not frozen, see also Section 6.2.

5.3.7 Handling in safety assessment

This section gives a description of how the process of diffusion in the rock mass is handled, divided in two parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-3 and Table 5-4 are addressed. On a general note, the Fickian diffusion theory is recommended to be used throughout SR-PSU modelling. Sorption should be accounted for by using the apparent diffusivity D_a (m^2/s) in Fick's diffusion equations, where $D_a = D_e/(\varepsilon + \rho K_d)$.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

During this period, the evolution of the groundwater composition is not modelled. As the groundwater flows towards, and not from, the repository, retention of dissolved solids by way of matrix diffusion, is of no concern.

Periods of the temperate climate domain

During these periods, radionuclide release is expected to be ongoing from the repository, although at different rates and along different flow paths. Diffusion of solutes between flowing and stagnant water volumes is included in the computational code that models radionuclide transport, see Section 6.2.

In SR-PSU it has been decided not to model density driven flow (see Section 3.2). Therefore, the evolution of the groundwater salinity is not used as an input to hydrogeological modelling. Accordingly, diffusional transport between flow paths and stagnant water volumes are not modelled for this purpose. In the hydrogeochemical modelling during these periods, matrix diffusion is included in a one-dimensional representation of the flowpath (and its surrounding rock) in the computational code FASTREACT (Román-Ross et al. 2014).

Periods of the periglacial climate domain

As the permafrost reaches repository depth, water flow from the repository ceases. As the water in the fractures is frozen there is no diffusional exchange between fracture water and the rock matrix. As the water in the microporous system of the rock matrix freezes at lower temperatures than in the fractures, if it freezes at all, previously released radionuclides existing in the rock may diffuse further into the matrix even under permafrost conditions, see also Section 6.2. However, this effect is neglected in radionuclide modelling. In the hydrogeochemical modelling during these periods, matrix diffusion is included in a one-dimensional representation of the flowpath and its surrounding rock (Román-Ross et al. 2014).

Periods of the glacial climate domain

As the ice sheet is warm-based during periods of the glacial climate domain, should such occur during the assessment period, liquid phase diffusion is possible, as the water in the bedrock is unfrozen. During these periods, solute transport/retention in the geosphere by way of matrix diffusion is neglected in SR-PSU.

Earthquakes

Earthquakes may reactivate previously sealed or partly sealed fractures, or open up or even expand fractures in the previously intact rock matrix. In any case, diffusional exchange between flow paths in these "new" fractures and surrounding stagnant water volumes is accommodated by the same process as described in the rest of this section. In earthquake scenarios, solute transport/retention in the geosphere by way of matrix diffusion is neglected in SR-PSU.

Handling relative to geosphere variables

Temperature in bedrock

The natural variability in the effective diffusivity, as result of differences in temperature, is included in the uncertainty range of D_e data (**Data report)**. This range is assumed to be valid for all time periods, climate domains, and events. For interpretation of in situ resistivity logs in derivation of formation factors as input data (inverse modelling), temperature viscosity corrections are implicitly included in the data handling.

Groundwater flow

As mentioned above, density driven flow is not modelled in SR-PSU.

Groundwater pressure

As water is an incompressible medium, the groundwater pressure does not influence liquid phase diffusion.

Gas phase flow

No detailed gas phase flow modelling is performed in SR-PSU (see Section 3.3).

Repository geometry

There is no need to address diffusion from the point of view of repository geometry.

Fracture and pore geometry

The pore geometry of the rock matrix affects the effective diffusivity. Accordingly, diffusivities based on site specific data are provided (**Data report**) to be used in modelling activities in SR-PSU. The effective diffusivity is assumed to be constant in time, within its uncertainty range, during the entire repository evolution.

Solute transport modelling adheres to the findings of Crawford and Sidborn (2009) concerning channelling, and which part of the fracture plane allows for diffusive exchange between the flowing water and the rock matrix. Accordingly, the entire fracture plane is accounted for when assessing the contact area (flow-wetted surface) in radionuclide transport modelling.

The fracture and pore geometry is assumed to be invariable throughout the assessment time frame. This means that possible precipitation in the porous system as result of an alkaline plume, which may alter the fracture and pore geometry, is neglected. Natural analogue studies (see Section 5.3.5) support this handling. The matter is also discussed in Sections 5.4 and 5.5).

Rock stresses

Natural variability of the effective diffusivity, as result of differences in rock stress affecting the rock matrix, is included in the uncertainty range of D_e data suggested in the **Data report**. This range is assumed to be valid for all time periods, climate domains, and events.

Matrix minerals

The processes of alteration, precipitation and dissolution of the rock matrix minerals under natural conditions are considered to be too slow, relative to the assessment time frame, to be of importance for matrix diffusion.

Fracture minerals

Fracture minerals (or fracture coatings) are assumed not to hinder diffusion of solutes from the fracture into the rock matrix, by other mechanisms than sorption. In practise this means that the effective diffusivity of fracture coatings is pessimistically assumed to be identical to that of the underlying rock matrix in modelling activities involving matrix diffusion.

Groundwater composition

The diffusivity of a solute depends on its properties, on the properties of the surrounding fluid, and on the properties of the surrounding matrix. The groundwater and pore water compositions affect the properties of the solute, if its speciation changes with changing chemical conditions, and of the surrounding fluid. Therefore, estimating individual diffusivities for elements/species/radionuclides is beyond the scope of the safety assessment. Instead, the uncertainty range (or distribution) given for the effective diffusivity in the **Data report** should encompass uncertainty due to speciation, fluid properties, and matrix properties. Generally the uncertainty due to matrix properties overshadows uncertainty due to the former issues.

In SR-PSU, groundwater composition modelling focuses on the flowing water in fractures (Román-Ross et al. 2014). The composition of this water is largely dependent on diffusive exchange between the flow path and the surrounding stagnant water. This diffusive exchange is included in a one-dimensional representation of the flowpath (and its surrounding rock) in the computational code FASTREACT which is applied (Román-Ross et al. 2014).

Gas composition

No detailed gas composition modelling in the geosphere is performed in SR-PSU.

Structural and stray materials

The integrity of structural and stray materials is not accounted for in SR-PSU. The impact on groundwater composition by structural and stray materials is assumed to be dwarfed by the impact of similar materials in the waste and barriers.

Saturation

In SR-PSU, the entire rock volume is assumed to be fully saturated. During the excavation, operation, and re-saturation phase, partly unsaturated conditions may apply in the host rock directly adjacent to rock caverns. However, no modelling involving diffusion is made for this period.

5.3.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Diffusion/matrix diffusion is a well-known process that is described in detail and can be fairly well modelled. Throughout decades, 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. Concerning the scale of the connected porosity, recent evidence (e.g. Löfgren and Neretnieks 2006, Crawford 2008, Waber et al. 2009a, b) strongly suggest that the porous system of the repository host rock generally is connected on all scales relevant for a safety assessment.

Matrix diffusion has become increasingly important for safety assessments in terms of modelling of groundwater compositions, and in some cases groundwater flow. This modelling has proved to be sensitive, at least to a certain extent, to the exchange of the groundwater main constituents (such as Na^+ and Cl^-) between flow paths and the rock matrix. These constituents do not exist in tracer concentrations, but in relatively high concentrations. In the pore water system, electrostatic interactions between the ionic solutes, and also the charged mineral surface of the rock matrix, are of concern. It could be questioned, on conceptual grounds, how well Fickian diffusion theory represents such a highly charged multicomponent system. A diffusion theory perhaps better equipped to handle such a system is the Maxwell–Stefan theory (Krishna and Wesselingh 1997). However, it is not suggested to take such an approach in SR-PSU, as the robustness of using this theory in the crystalline rock system first needs to be demonstrated. As the diffusion theories do not fully represent the studied system, the modelling must to a certain degree rely on empiric knowledge, where uncertainty is handled by sensitivity analysis.

Model simplification uncertainties

Matrix diffusion is generally modelled as diffusion in a homogenous medium, which must be seen as a model simplification. However, this discrepancy is of greater consequence for tracer test scale than for safety assessment scale. As stated in the previous subsection, using Fickian diffusion in the crystalline rock system is also a model simplification. Modelling simplifications in hydrogeochemical modelling include using a one-dimensional representation of the flowpath (and its surrounding rock) in FASTREACT (Román-Ross et al. 2014).

5.3.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.4 Speciation and sorption

5.4.1 Overview/general description

The geosphere processes “speciation and sorption” are discussed in this section in a broad sense, while specific aspects of *radionuclide* speciation and sorption in the geosphere are discussed later in Section 6.1. It must be pointed out, however, that speciation and sorption processes are of much more importance for radionuclides than for other types of groundwater solutes when evaluating the long term safety of nuclear repositories.

The term “sorption” is a broad concept that describes the processes by which dissolved solutes are sorbed (adsorbed or absorbed) on or in another substance (IUPAC 1997). In the context of radionuclide transport processes relevant for safety assessment, however, adsorption of dissolved species to mineral surfaces is mainly by way of electrostatic and covalent chemical bonding (surface complexation). Groundwater solutes are frequently in the form of ionic, charged species and will tend to sorb on mineral surfaces that possess a net charge of opposite sign. Such interactions are well described in the scientific literature (e.g. Stumm and Morgan 1996) and the most important interaction mechanisms are considered to be ion-exchange (a purely electrostatic adsorption process) and surface complexation (involving covalent bonding to chemically reactive surface groups).

Sorption can take place directly on the outer surfaces of flow-bearing fractures or on grain-boundary surfaces and microfractures within the rock matrix, where the porewater is effectively stagnant. Sorption can also take place on other materials, such as secondary clay minerals in fracture-surface coatings. Generally, sorption processes result in the retardation of solute transport along a flow path, although when radionuclides sorb on mobile solid materials such as colloids, the effectiveness of the retardation may decrease, see also Section 5.9. There are other processes apart from sorption, such as precipitation and co-precipitation, which can give rise to additional retardation effects for transported solutes, as described in Section 5.6. However, owing to the difficulties in adequately quantifying and modelling these processes, they are not usually considered to contribute significantly to retardation in safety assessments.

The consideration of mineral precipitation/dissolution and the formation of solid solutions (i.e. co-precipitates) is, however, crucial for establishing relevant background concentration ranges for stable and naturally occurring radioactive isotopes which can influence the sorption of their radioactive, repository derived counterparts. This is particularly important for solutes such as caesium, strontium, and uranium. Consideration of the background concentrations of stable and naturally occurring radioactive isotopes is important for the assessment of sorption properties owing to the frequently non-linear nature of radionuclide sorption isotherms. In the case of radium, natural background levels of the radionuclide are sufficiently high that this largely determines the concentration range in which sorptivity of the nuclide is to be assessed. Co-precipitation of radium and barium as a solid solution in barite is well known and, under most environmental conditions, is expected to exert an important control on the concentration range of radium present in groundwater owing to the low solubility of barite and its ubiquitous nature (Bruno et al. 2007). Although such processes are carefully considered in SR-PSU during the selection of K_d data (Crawford 2013), no attempt is made in SR-PSU to attribute additional retention in the geosphere transport modelling (**Radionuclide transport report**) arising from these processes on account of the difficulty of demonstrating that they provide a reliably quantifiable retardation effect.

Depending on the process in question, the strength of the sorption is highly dependent on the chemical properties of the individual ions and the presence of complexing agents and other dissolved solutes in the groundwater that may compete for sorption sites. It is, therefore, essential to know the redox conditions, groundwater pH, and concentration of complexing agents, such as carbonate or isosaccharinate, in order to predict sorptivity. Certain chemical elements (e.g. uranium, neptunium, and plutonium) are sensitive to redox conditions, whereas others (e.g. caesium, strontium, and thorium) are generally insensitive to the redox conditions in the groundwater. For the elements that exhibit such sensitivity, the chemical valency of the dissolved solute is controlled by the redox state of the groundwater, which affects the propensity of the solute to form chemical bonds with mineral surface groups and undergo surface complexation.

Complexation in the aqueous phase can reduce the sorptivity of solutes, although in other instances the sorptivity can actually be increased (e.g. bidentate sorption of uranyl carbonato complexes (Bargar et al. 1999)). The magnitude of the effect depends upon the chemical properties of the solute concerned and the types of complexing agents present and their properties. The solution chemistry of simple complexing agents, such as dissolved carbonate, is well described theoretically and can be accounted for with relative ease in the aqueous phase. However, the impact on sorptivity when participating in sorption reactions is often less well characterised. The presence of dissolved carbonate, for example, can have complex direct and indirect effects that are difficult to predict *a priori*.

More complex ligands such as humic and fulvic substances can also be accounted for, although they are generally associated with decay of cellulosic or other organic materials and are frequently of concern in surface and near-surface environments. Under high pH conditions as could be expected to occur in the SFR repository, isosaccharinic acid (a decay product of cellulosic materials) may constitute a strong aqueous complexing ligand. Depending on its concentration, this may both enhance the release of radionuclides from SFR as well as reduce the sorptivity of transported radionuclides along transport paths in the geosphere. 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 depth, these substances are considered to be of only limited importance, although in near surface aerobic environments this could potentially have a non-negligible impact on radionuclide sorptivity.

In connection with ion exchange, the salinity of the water is of great importance. High salinity reduces the sorption of, for example, caesium and strontium by way of competitive effects, involving ion-exchange sorption of other cations in the groundwater.

The different minerals participating in sorption reactions have different capacities for adsorption. Clay minerals and iron oxyhydroxides, for example, have a large sorption capacity, whereas quartz and feldspar tend to sorb very weakly. In granitic rocks, it is typically dark minerals such as biotite, or its alteration product chlorite, as well as hornblende, which are thought to have the strongest affinity for sorption. The sorption of caesium and strontium, for example, is known to be strongly concentrated to biotite and chlorite (micas) which, being phyllosilicate minerals, have a large capacity for ion-exchange sorption (e.g. Torstenfelt et al. 1982, Huitti et al. 1998). Uranium and neptunium also have an affinity for the iron-rich dark minerals (Kienzler et al. 2009), possibly due to surface complexation sorption on frayed edge sites of micas combined with reduction to the more strongly sorbing tetravalent state. The surface complexation sorption of nickel, plutonium and americium, on the other hand, appears to be less specific, although autoradiographic studies do suggest heterogeneous distribution of sorption (Pinnioja et al. 1984) with sorption concentrated on minerals possessing high surface areas, such as biotite/chlorite and hornblende.

Although sorption of solutes, including radionuclides, is generally reversible in a thermodynamic sense, the incorporation of metal ions into mineral lattices can result in an effectively irreversible immobilisation. However, owing to the dynamic equilibrium of most common mineral phases likely to incorporate radionuclides, irreversible immobilisation is not always verifiable, and such retardation processes are usually neglected in safety assessments.

Although the master variables pH, redox, and concentration of complexing ligands in the groundwater largely determine the speciation (distribution of an element amongst different chemical species) of chemical elements, temperature and pressure also play a minor role by way of the effect that these variables can have upon the thermodynamics of chemical reactions. The importance of chemical speciation in safety assessments lies in its impact on the geochemical retention and immobilisation reactions likely to occur and their consequences for radionuclide mobility.

The existence of an alkaline pH plume (i.e. OPC leachate, Ordinary Portland Cement) emanating from the SFR repository may influence the retardation of radionuclide transport in a number of ways. The high pH plume may enhance sorption by promoting sorption reactions involving hydrolysed radionuclide species. At the same time it may reduce sorption by way of increased hydrolysis of radionuclide species in the aqueous phase. The net effect depends on the balance between the binding to surface reactive groups and the binding by the hydroxyl ligand in the aqueous phase. Sorption of some actinides and lanthanides may also be significantly reduced at high pH in the presence of an atmospheric partial pressure of carbon dioxide due to complexation by dissolved carbonate ligands (i.e. HCO_3^-). At the same time, sorption may be promoted by increased carbonate concentrations due to ternary sorption reactions involving radionuclides and carbonate. Similarly to the reactions involving hydroxyl-surface complexes, the net effect depends on the balance between binding by free carbonate ligands in the aqueous phase and reactive groups in the solid surfaces. In the groundwater surrounding the SFR repository, however, equilibrium with a fixed partial pressure of CO_2 is unlikely and the dissolved carbonate concentration is then limited by calcite equilibrium. In the presence of elevated Ca^{2+} concentrations, calcite precipitation will scavenge carbonate from the aqueous phase, giving very low effective CO_2 partial pressures (on the order of 10^{-12} atm, or less).

Another way in which an alkaline pH plume may influence retardation of migrating radionuclides is by way of altering the material properties of the rock matrix. In the immediate vicinity of the repository, high pH conditions may promote the dissolution of quartz and precipitation of secondary Ca-silicate crystalline or gel phases. Similarly the dissolution of plagioclase may result in the precipitation of Mg-saponites. Since these secondary minerals typically have a larger molar volume than the primary quartz dissolved from the rock matrix, the net effect is a decrease in porosity, both in the rock matrix and in the fractures immediately adjacent to SFR. Although this is an effect which might be expected to primarily influence the rock matrix effective diffusivity, it may also influence sorptivity, as secondary precipitates would cover the surface of other minerals in such a way that the overall sorptive retardation effect is altered.

Such processes are difficult to predict owing to uncertainty concerning boundary conditions. The high pH of an OPC plume would be expected to decrease with time as the cement ages and easily mobilised basic cations are depleted. Additionally, if mixing occurs with non-OPC affected groundwater, then neutralisation reactions accompanied by calcite precipitation will occur. Precipitation of calcite due to diffusive mixing of different groundwaters in the rock matrix is not expected to result in a significant porosity reduction in the rock matrix since it is limited by the initial inventory of dissolved Ca^{2+} and carbonate in the porewater which is vanishingly small relative to the potential volumes of calcite that can be precipitated. This is not the case for secondary precipitation resulting from dissolution of quartz and plagioclase since these primary minerals are present in effectively limitless quantity in the rock matrix. On the other hand, if hydrodynamic mixing and neutralisation in the advective flow space significantly reduces the pH over a sufficiently short distance from the repository, then dissolution of primary matrix minerals may decrease to such a low level that pore clogging by secondary mineral precipitates can be neglected throughout most of the geosphere along major transport paths.

5.4.2 Dependencies between process and geosphere variables

In this section, dependencies between the speciation and sorption processes and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-5 outlines how the processes are influenced by the defined geosphere variables, while Table 5-6 outlines how the processes influence the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is relevant. The influence between the process and each geosphere variable is elaborated upon below.In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. In Section 5.4.7, this handling is elaborated upon in a discussion provided by the SR-PSU team.

Table 5-5. Direct influences of defined geosphere variables on the processes "sorption and speciation" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation and saturation, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domains, EQ = Earth quake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.4.7)
Temperature in bedrock	Yes. A temperature dependence exists.	All	The impact of temperature on sorption processes is currently neglected owing to a lack of data. Impacts, however, are expected to be relatively minor relative to their uncertainties.
Groundwater flow	No, but indirectly through: Groundwater composition.	All	–
Groundwater pressure	Not significantly.	All	–
Gas phase flow	No, but indirectly through: Groundwater composition.	All	–
Repository geometry	No.	All	–
Fracture and pore geometry	Yes. Fracture and pore geometry determines sorption surface area, and accessibility to this area.	All	Site-specific porosities, BET surfaces and stress effects considered in the selection of K_d (**Data report**, Crawford 2013).
Rock stresses	No, but indirectly through: Fracture and pore geometry.	All	–
Matrix minerals	Yes. Mineralogy is important for sorption mechanisms in matrix.	All	Site-specific minerals and BET surfaces considered in the selection of K_d values (Crawford 2013).
Fracture minerals	Yes. Mineralogy is important for sorption mechanisms on fracture surface.	All	Sorption on fracture surfaces neglected in SR-PSU (**Radionuclide transport report**).
Groundwater composition	Yes. Redox, pH, salinity, etc affects K_d.	All	K_d data, with uncertainty ranges, are assumed to be approximately adequate, or conservative, for the in situ groundwater composition ranges (Auqué et al. 2013). Different K_d values given for different speciation, as result of different redox potential range (Crawford 2013).
Gas composition	No, but indirectly through: Groundwater composition.	All	–
Structural and stray materials	Yes. Sorption may take place on cement materials. Also indirectly through: Groundwater composition.	All	Sorption on cementitious materials in rock matrix (grouting materials, rock reinforcements) is not considered in SR-PSU. Changes in sorption upon contact with cementitious materials are considered, see Section 5.8.
Saturation	Yes. By affecting the surfaces accessible to sorption.	E/O/S	Radionuclide release during this period is not expected, due to direction of hydraulic gradient towards the repository.
		T/P/G/EQ	Sorption is considered for fully saturated conditions only.

Explanation of Table 5-5

Temperature in bedrock

Temperature influences all chemical reactions that are likely to occur in groundwater as well as surface chemical processes (sorption, ion-exchange and dissolution/precipitation). As a general rule, equilibrium chemical reactions described as being exothermic (producing heat) are promoted by reduced temperatures while endothermic reactions are hindered. Temperature can also have an indirect impact on sorption by altering the species distribution of the solutes in groundwater. By altering the thermodynamic conditions for solution speciation reactions, competitive effects are therefore subtly altered. The direct effect of temperature on reaction equilibrium constants may be estimated using the Van't Hoff equation (e.g. Langmuir 1997), provided reliable reaction enthalpy data are available. At present there is little data of sufficiently reliable quality to extrapolate sorption K_d values to temperatures differing from standard laboratory operating temperatures (typically, 22–25°C). Temperature effects are, however, not expected to have a sufficiently large impact on sorption processes for the purposes of SR-PSU.

It is currently possible to extrapolate some aqueous phase chemical reactions (i.e. governing groundwater speciation) and certain precipitation/dissolution reactions to temperatures other than 25°C. The results are, however, subject to uncertainty owing to internal inconsistencies and uncertainties in the thermodynamic databases used for such calculations.

Groundwater flow

Groundwater flow may indirectly affect speciation and sorption, by way of affecting the groundwater composition.

Groundwater pressure

The groundwater pressure has a negligible direct effect on speciation and sorption, by way of affecting the equilibrium constants.

Gas phase flow

Gas phase flow may indirectly affect speciation and sorption, by way of affecting the groundwater composition upon dissolution/degassing.

Repository geometry

The repository geometry has no direct effect on either speciation or sorption.

Fracture and pore geometry

Fracture and pore geometry determines sorption surface area, and accessibility to this area via advection or matrix diffusion.

Rock stresses

Rock stresses should not directly affect speciation and sorption, but there may be an indirect effect through fracture and pore geometry.

Matrix minerals

The mineralogy is important for the sorption mechanisms, as well as for the sorption capacity.

Fracture minerals

The mineralogy is important for the sorption mechanisms, as well as for the sorption capacity.

Groundwater composition

The fracture groundwater (or the rock matrix pore water) composition greatly affects sorption as it affects the speciation of the sorbing species, as well as the sorption sites through pH effects, salinity effects, etc.

Gas composition

Gas phase flow may indirectly affect speciation and sorption, by way of affecting the groundwater overall composition upon dissolution/degassing.

Structural and stray materials

Sorption may take place on cement materials, such as grout. Sorption may also be affected indirectly by structural and stray materials, since their degradation can influence groundwater pH and create secondary minerals in fractures etc.

Saturation

Saturation has a direct effect by affecting the surfaces accessible to sorption.

Table 5-6. Influences of the processes "sorption and speciation" on defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in 5.4.7)
Temperature in bedrock	No.	All	–
Groundwater flow	No, but indirectly through: Groundwater composition.	All	–
Groundwater pressure	No.	All	–
Gas phase flow	No, but indirectly through: Groundwater composition.	All	–
Repository geometry	No.	All	–
Fracture and pore geometry	No.	All	–
Rock stresses	No.	All	–
Matrix minerals	No.	All	–
Fracture minerals	No.	All	–
Groundwater composition	Yes. Uptake and release of solutes controls concentration in water phase.	All	Sorption is taken into account when modelling radionuclide concentrations. Sorption is not explicitly accounted for when modelling groundwater composition but its effects are included in the groundwater composition data from site investigations reported in SKB (2011).
Gas composition	No, but indirectly through: Groundwater composition.	All	–
Structural and stray materials	No.	All	–
Saturation	No.	All	–

Explanation of Table 5-6

Temperature in bedrock

Changes in speciation or sorption do not affect the bedrock temperature.

Groundwater flow

The effect of speciation and sorption on groundwater composition (thus also water viscosity and density) is too small to affect the groundwater flow.

Groundwater pressure

Neither the speciation nor sorption affects the groundwater pressure.

Gas phase flow

In principle, sorption may affect groundwater composition and indirectly by dissolution, degassing the gas phase flow. However, the effect is too small to be of significance.

Repository geometry

Speciation or sorption does not affect the repository geometry.

Fracture and pore geometry

Speciation or sorption does not affect the pore space or fracture geometry

Rock stresses

Speciation or sorption does not affect the stress situation of the bedrock.

Matrix minerals

Sorption may change the surface properties of the matrix minerals, such as surface charge, but not their composition.

Fracture minerals

Sorption may change the surface properties of the fracture minerals, such as surface charge, but not their composition.

Groundwater composition

Speciation, and the partitioning between solutes and sorbed species affects the groundwater composition.

Gas composition

The gas composition may be affected indirectly since water phase and gas phase concentrations are related by thermodynamic relations.

Structural and stray materials

Speciation and sorption in the geosphere do not have a significant effect on structural and stray materials.

Saturation

Sorption and speciation should not affect the degree of saturation in any significant way.

5.4.3 Boundary conditions

Speciation and sorption are small scale process that are mainly determined by the groundwater overall composition and mineralogy of the fracture minerals and matrix minerals, or the properties of other solids present (e.g. colloids). The groundwater overall composition both determines the speciation of the solutes and the functional groups at the solid surfaces. To a lesser extent the sorption/desorption reactions are bounded by the temperature and pressure.

5.4.4 Model studies/experimental studies

Sorption of aqueous species on solids can be quantified empirically using a K_d approximation or described using mechanistic modelling approaches that include speciation in the groundwater. The K_d concept simply describes the partitioning ratio of sorbed to dissolved solute without any specific consideration of reaction mechanisms or speciation. More elaborate, isotherm-based approaches attempt to capture non-linearities of sorptivity with changes in solute surface loading and competitive effects, although they are still based upon largely empiric reasoning without reference to specific sorption mechanisms. Mechanistic modelling approaches are based upon a thermochemical formulation (thermodynamic sorption models, or TSM's). Surface-complexation and ion-exchange models fall into this latter category.

Sorption of a number of radionuclides (isotopes of Cs, Sr, Am, Ra, Ni, U, Np) has been studied as part of the transport properties in the site investigations at Forsmark and Laxemar (SKB 2008d, 2009). Other experimental, radionuclide-specific studies of sorption are reported in the literature and have been used both for SR-PSU and in previous compilations of sorption properties (e.g. Crawford et al. 2006, Carbol and Engkvist 1997, Stenhouse 1995, Hakanen and Hölttä 1992). These are usually conducted as batch tests, where a radionuclide spiked groundwater (or simulated groundwater) volume is contacted with a geological sample (usually crushed) for a period of time ranging from days to months until an approximately equilibrium state is reached. Rock samples and water compositional ranges are chosen to represent the typical spatial variability for the repository site (usually this reflects a range of pH levels, redox states, ionic strengths and radionuclide concentrations). The change in the aqueous concentration of the radionuclide relative to its initial concentration provides an indication as to the extent of sorption, provided precipitation or colloid formation can be ruled out. Column tests with flowing water can also be used to estimate the sorption, although interpretation is additionally complicated by the need to simultaneously account for more complex transport processes. In the field, attempts have been made to estimate sorption directly by determining the distribution of a tracer between fracture surfaces and equivalent groundwater in boreholes (e.g. Landström and Tullborg 1990) although interpretation is difficult (e.g. McKinley and Alexander, 1992, 1993a, b). Transport experiments with sorbing tracers in the field can also be used to estimate the strength of the sorption process (e.g. Löfgren et al. 2007, Nilsson K et al. 2010, Smith et al. 2001, Alexander et al. 2009). In addition, sorption properties can be evaluated from in-diffusion and through-diffusion experiments in intact rock pieces (e.g. Byegård et al. 1998, Widestrand et al. 2010).

Provided the sorption is an approximately linear, reversible process, a distribution coefficient, K_d, for the particular water chemistry in question can be estimated. For radionuclides, given the low concentrations that are of interest, the assumption of linearity is usually satisfied, or otherwise incorporated in the overall range of uncertainty estimated for the K_d value, and the assumption of equilibrium is met if the sorption process has a characteristic timescale that is much shorter than the timescale for advective transport. The use of K_d entails a simplification of what is, in reality, a very complex set of processes. Models that take into account non-linear sorption or non-equilibrium conditions exist, although they are seldom used in safety assessments owing to difficulty of implementation in an adequate fashion.

5.4.5 Natural analogues/observations in nature

Sorption as a reversible equilibrium process is difficult to observe directly in nature in an unambiguous fashion owing to the very low immobilised concentrations characterising the process. However, other immobilisation processes, such as precipitation, are easier to observe macroscopically and can be readily studied in geological samples (see Sections 5.5 and 5.6). A compilation of studies on natural analogues regarding the mechanisms controlling the aqueous concentrations and speciation of several elements is given in Bruno et al. (2002).

Sorption can, in principle, be studied by examining the immobilisation of tracer solutes within rock samples retrieved in post-mortem evaluations of tracer experiments. The excavation of the rock volume involved in tracer tests can also be performed in conjunction with resin injection which allows the flow space structure to remain intact thereby giving additional information concerning fracture aperture and porosity distributions (see e.g. Möri et al. (2003a) and the review of SKB related tracer studies in Löfgren et al. (2007) and Byegård et al. 2014)).

5.4.6 Time perspective

For most radionuclides, sorption processes are considered to be very fast compared with the timescale for advective transport in fractured rock. This means that dynamic sorptive equilibrium between the rock and aqueous phase can be assumed to prevail under natural conditions. Processes that lead to incorporation of radionuclides in mineral lattices are much slower than ion exchange and surface complexation and cannot always be considered to be in an equilibrium state. However, these processes are not relied upon directly in the safety assessment and may be considered to be processes that give rise to additional, although unquantified, retardation.

5.4.7 Handling in the safety assessment

In this section, the SR-PSU team gives recommendation on how to handle the processes of speciation and sorption. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-5 and Table 5-6 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation 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 groundwater flow is towards the vaults. Speciation and sorption in the geosphere are not included for this period in SR-PSU, as no geochemical modelling for this period is performed and no liquid phase radionuclide transport is expected to occur.

Periods of the temperate climate domain

For radionuclide sorption, it is assumed that a simplified linear equilibrium model (constant K_d) is applicable for safety assessment, see also Chapter 6. This approach implies that geochemical conditions are sufficiently time invariant that the simplified modelling approach is valid and that retention processes such as surface precipitation and co-precipitation are not considered to contribute towards retardation in the safety assessment. Details of the modelling of radionuclide transport in the geosphere, where speciation and sorption is included, are described in the **Radionuclide transport report**.

In order not to overestimate sorption in connection with possible changes in water chemistry, cautiously pessimistic distribution coefficients are assigned (Crawford 2013). In SR-PSU, Craword (2013) has derived a set of K_d values for ion-exchanging solutes for different site-specific conditions (groundwater compositions during different climate condtions, i.e. ranges of different major ion compositions) as defined by Auqué et al. (2013). For radionuclides that sorb principally by way of a surface complexation mechanism, best estimate K_d values are provided for the entire span of expected groundwater compositions likely to be encountered under oxidising and reducing conditions (Crawford 2013). The speciation of particular redox-sensitive radionuclides is assessed on an individual basis using the groundwater compositions established by hydrogeochemical modelling as a basis. Uncertainty distributions for radionuclide-specific K_d values are provided that include both experimental uncertainty and uncertainties regarding the geochemical environment of the rock. For further discussion of parameter values in SR-PSU, the reader is referred to Crawford (2013).

Sorption is not explicitly accounted for when modelling groundwater composition in SR-PSU (Román-Ross 2014). However, the process is to some extent incorporated in the modelling, as it uses input data based on groundwater composition measurements in the site investigations reported in SKB (2013b).

Periods of the periglacial climate domain

The same approach as outlined above for periods of temperate conditions is used for periods of the periglacial climate domain. K_d values are chosen to represent the relevant geochemical conditions characterising these climate domains.

Periods of the glacial climate domain

The same approach as outlined above is used for periods of the glacial climate domain. K_d values are chosen to represent the relevant geochemical conditions characterising these climate domains (Auqué et al. 2013). During glacial periods the intrusion of oxygen-rich meltwaters down to the SFR can not be excluded. As a result, oxidising conditions may prevail in the flow paths (fractures), falling outside the range for which K_d data are provided for some elements. Under such conditions these elements are assumed to be non-sorbing, see Crawford (2013). However, non-sorbing cases for the geosphere are applied as a cautious assumption for radionuclide transport calculations (**Radionuclide transport report**).

Earthquakes

In case of an earthquake, this is handled by short-circuiting the geosphere and not accounting for any radionuclide retention, see the **Radionuclide transport report**. In terms of groundwater composition evolution, the earthquake is assumed not have a significant impact.

Handling relative to geosphere variables

Temperature in bedrock

By using the K_d approach, temperature effects are neglected owing to lack of internally consistent data sets. However, this is a minor source of uncertainty.

Groundwater flow

There is no direct dependency between sorption and groundwater flow that needs to be handled in SR-PSU modelling.

Groundwater pressure

The influence of groundwater pressure on the equilibrium constants in the groundwater and between sorbed and de-sorbed solutes is neglected, as it has little significance compared with other influences.

Gas phase flow

No detailed gas phase flow modelling is made for the geosphere.

Repository geometry

There is no direct dependency between sorption and repository geometry that needs to be handled in SR-PSU modelling.

Fracture and pore geometry

The geometry of flow paths would affect the amount of surface sorption available. However, retardation on fracture surfaces is neglected in SR-PSU radionuclide transport modelling (see Section 6.2). Concerning entities related to the micropore geometry; site-specific porosities, BET surfaces, and stress effects are considered in the selection of K_d, see Crawford (2013).

Rock stresses

Potential changes in rock stresses should not affect the sorption (by way of enhancing/restricting access to mineral surfaces) to such degree that it should be significant for the safety assessment. Therefore, potential changes in rock stress compared to present day situation are not considered when assigning K_d values.

Matrix minerals

The general mineralogy of the rock mass surrounding fractures is of importance for the radionuclide sorption capacity. Where available, sorption data have been obtained on site specific rock. Where such data have not been available, to the greatest extent possible the chosen data represent similar rock types as at the Forsmark site. For detailed information, see Crawford (2013).

Fracture minerals

In radionuclide transport modelling sorption on fracture surfaces is not generally accounted for (see Section 6.2).

Groundwater composition

The fracture groundwater (or the rock matrix pore water) composition greatly affects sorption as it affects the speciation of the sorbing species, as well as the sorption sites through pH effects, salinity effects, etc.

The groundwater composition during different climatic cases and based on site data (Auqué et al. 2013) is explicitly considered when selecting the sorption data (Crawford 2013) used to model radionuclide transport in the geosphere (**Radionuclide transport report**).

Gas composition

No detailed gas composition modelling is made for the geosphere.

Structural and stray materials

The influence of structural and stray materials on speciation and sorption is neglected in SR-PSU modelling. This is justified as the same materials exist in much higher quantities in the rock vaults of the repository (see the **Waste process report** and the **Barrier process report**). Interferences with structural and stray materials are accordingly overshadowed.

Saturation

Throughout repository evolution, fully saturated conditions are assumed in the rock mass. In this respect the very short initial saturation period is neglected.

5.4.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Since sorption is a collective term for a number of different processes, modelling simplifications imply conceptual uncertainties even though the underlying mechanisms and processes are well understood. The use of the simplification implied by the use of a constant K_d is conceptually and practically attractive, although the validity of this approach can be questioned under certain specific conditions when the prerequisites of the concept (temporally invariable groundwater composition, linearity, reversibility and equilibrium) are not strictly fulfilled. The prerequisites in terms of linearity and equilibrium are generally met for the conditions that apply in the safety assessment, even if competition for sorption sites by major ions may imply non-linearity for some elements. Although groundwater compositions cannot realistically be expected to be static over very long timescales (see for example Auqué et al. 2013), K_d values are chosen to cautiously over-predict radiological risk where this uncertainty does exist. Thus, the validity of the concept does not in itself entail an uncertainty factor, given the purpose of the safety assessment and provided conditional K_d values are chosen in such a way that retardation is not overestimated.

There are still a number of outstanding issues concerning interpretation of experimental laboratory data that need to be considered in greater detail before concluding that the compiled K_d values are, indeed, cautious in a performance assessment framework. The formal handling of these uncertainties typically results in expanded ranges of statistical uncertainty which may not be fully representative of the systematic variability of the underlying process with regard to mechanistic dependencies on physicochemical conditions.

Many effects related to the use of crushed rock, effects of contact time, and effects of water composition are not well understood at present. Apart from these issues related to macroscopic data representativity, there is still considerable uncertainty concerning specific mechanisms underpinning sorption processes owing to a lack of data (i.e. internally consistent thermodynamic data for mechanistic modelling, characterisation of mineral phases dominating sorption processes, and spectroscopic confirmation of postulated sorption mechanisms). As a direct consequence of this, there is still considerable uncertainty concerning how best to extrapolate sorption properties derived from laboratory experiments conducted on crushed material to apply to intact rock under *in situ* stress conditions and possibly differing groundwater compositions. It is further noted that even measurements on whole rock pieces in the laboratory may be biased due to mechanical damage effects and possibly non-representative groundwater compositions.

Model simplification uncertainties

The representation of sorption using a conditional K_d approach implies some particular uncertainties in addition to the data interpretation issues outlined above. It should be noted that these forward modelling uncertainties would exist even with perfect knowledge of the mechanistic dependency of the conditional K_d value on physicochemical conditions. These uncertainties are related to the conceptualisation of the reactive transport process itself in safety assessment codes and ideally should be considered as a separate issue to that of sorption data interpretation. It is difficult to completely disassociate these issues, however, since consideration of the subsequent modelling simplifications, by necessity also guides the selection of appropriate K_d data in the first place. Acknowledging this, the K_d values are chosen cautiously with regard to the dynamics of the particular scenarios being modelled and thus do not provide a true representation of the transport mechanisms as they actually occur. Also, the fact that immobilisation processes such as precipitation/dissolution and solid solution formation (co-precipitation) and subsequent remobilisation if chemical conditions change are not included implies that realism is lost.

Sorption modelling based upon site-specific data is used to inform the selection of K_d values for ion exchanging radionuclides. Sorption by way of surface complexation can theoretically be described with mechanistic modelling approaches. These models are general and based upon well-founded theoretical concepts, although they require internally consistent and robust thermodynamic data sets for aqueous speciation, for the sorbing substances and for the minerals involved in the sorption process. Such modelling has been used in a supporting role in SR-PSU to discuss possible effects of a high pH plume on K_d ranges (see Crawford 2013), although the predictions cannot be regarded as being anything more than speculative. Although great advances have been made in recent years with regard to thermodynamic modelling of safety assessment relevant radionuclides on single minerals and simplified mineral assemblages (NEA 2001, 2005), the state of the art is deemed insufficiently mature for direct quantitative application within safety assessment modelling for granitic rock.

5.4.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. All supporting references are either peer-reviewed articles or documents which have undergone factual review. The most prominent supporting references are Crawford (2010, 2013), whereof the former is a dedicated SR-PSU report.

5.5 Reactions groundwater/rock matrix

5.5.1 Overview/general description

Stagnant groundwater with a long residence time, like preglacial, will eventually approach chemical equilibrium by reactions with the different minerals in the bedrock. However, most reactions between water and minerals are so slow that complete equilibrium will never be reached, at ambient temperatures, even if the water's flux in the bedrock is very slow. If there is a considerable groundwater flow, a groundwater far from equilibrium may be introduced, which can by advection of solutes in the groundwater 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. Alteration and larger porosity of the rock minerals as demonstrated in Forsmark usually occur at short distances from the fracture surface (Sandström et al. 2010, Sidborn et al. 2010). However, locally the extent of the altered rock can be much greater, especially within modelled fracture zones where more than 40% of the total borehole length has been affected by alteration in the regional SFR model volume (Curtis et al. 2011).

Ever since the rocks at SFR were formed between 1.9 and 1.8 billion years ago (Hermansson et al. 2008), chemical reactions have affected the rock. During rock formation, fluids were released which contained residual products, such as excess chloride, sodium and calcium, that did not fit into the crystal lattices. This water is called juvenile. Remnants of these fluids are hosted in fluid inclusions and usually contain large quantities of dissolved salts (Waber and Smellie 2008). Furthermore, during events of fracturing and reactivation of existing fractures, fluids of different character and origin have circulated through the rock episodically in the area, resulting in different precipitates (Sandström and Tullborg 2009, Sandström et al. 2009).

Processes involving brine waters (salinity > 10 percent, i.e. 100 g/L TDS according to Frape and Fritz (1987)) are not present in the upper investigated 1000 metres in the Forsmark area (Laaksoharju et al. 2008b) and therefore not relevant for SFR-PSU (SKB 2013b).

The rates for the chemical reactions that take place in the groundwater vary widely. Reaction rates for different kinds of reactions have been compiled by Bruno (1997). The fastest are metal hydrolysis reactions, with half-lives ranging from microseconds to tenths of seconds. Then complexation between metals and organic ligands, with half-lives of minutes, whereas fulvic and humic binding reactions proceed about ten times slower. Redox reactions with an electron transfer take from tens of minutes to several years, whereas redox reactions that require changes in molecular structure have half-lives of several to thousands of years.

Reactions that include solid phases (minerals) are generally much slower than reactions that take place in the aqueous phase. Exceptions are ion exchange reactions, which proceed just as quickly as reactions in the aqueous phase. Dissolving hematite in water takes tens to tens of thousands of years, and dissolution of aluminium silicate takes tens of thousands to millions of years (e.g. Zhu 2005). However, there are reactions between solid phases and water that are considerable faster, e.g. dissolution and precipitation of calcite, which have half-lives of seconds to days.

However, the reaction rate is also strongly dependent on the chemical environment where the reaction occurs. Precipitation of iron(oxy)hydroxide takes from picoseconds up to tens of years, depending on the pH, redox conditions and iron concentrations in the groundwater.

At very high pH, which can occur in contact with concrete, the reaction rates for dissolution of silicate minerals in granitic bedrock are 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). At high pH, the secondary phases consist of calcium silicate hydrates (CSH), which are common in concrete. Zeolites form at lower pH.

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 minerals has proceeded episodically. A prerequisite for reactions to occur is presence of fluids which can transport reactants and products. Fluid–rock reactions have also affected the rock's porosity and its thermal properties. The effects have been greatest under metamorphic and hydrothermal conditions, when hot chemically aggressive water has passed through the flow paths in the rock, preferentially along the major deformation and fracture zones. Hydrothermal conditions (> 200°C) have not occurred in the uppermost kilometre in the Forsmark area since the Mesoproterozoic (i.e. during the last 1,000 million years) (Sandström et al. 2009). During hydrothermal events, primary minerals in the rock adjacent to fractures have been altered into secondary minerals (e.g. albite, chlorite, epidote, hematite), material has been dissolved resulting in increased porosity in the wall rock, dissolution of older fracture filling minerals has occurred and large quantities of fracture-filling minerals have been deposited in the fracture system (Sandström et al. 2009). The major process in the rock matrix during hydrothermal alteration is dissolution–precipitation along a moving interface, inwards to the rock matrix (Putnis 2002). 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, highly transmissive fracture zones.

During the late Palaeozoic (ca 400 to 250 million years ago), an overlying sedimentary cover increased the temperature at the present erosion level to 50–150°C in large parts of the Fennoscandian Shield during a period of at least hundred million years (Larson et al. 1999). Leaching of these sediments led to formation of saline waters which subsequently migrated downward and precipitated fracture minerals like calcite (with very saline fluid inclusions), pyrite and quartz in the bedrock fractures (Sandström and Tullborg 2009). Even though the water that passed through the rock at that time has disappeared, it can still influence the groundwater through dissolution of phases precipitated from this water along the fractures.

The minerals in the rock have a varying tendency to be altered or dissolved in groundwater. The same reactions probably take place in the rock matrix and in water-bearing fracture zones. The difference is mainly that the water in the matrix is stagnant and transport of reactants and reaction products takes place mainly by diffusion (Waber et al. 2009a, b). There is no sharp borderline between water-bearing fractures and the rock matrix where diffusion dominates (Section 5.3).

Human activities such as drilling may influence the groundwater composition by short-circuiting groundwaters with different hydrochemistry. However, such induced changes in groundwater composition would primarily affect the fracture filling minerals in the SFR-area and not the rock matrix minerals to any significant extent.

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.

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 reducing capacity available in the rock matrix at SFR exists mainly in the Fe(II)-bearing biotite, chlorite, amphibole, pyrite and magnetite. Biotite is, by far, the main reducing mineral in the rock matrix at SFR (Sandström and Stephens 2009, Curtis et al. 2011, Sidborn et al. 2010).

The measured 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

In this section, dependences between the groundwater/rock matrix reactions and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-7 outlines how the process is influenced by the defined geosphere variables, while Table 5-8 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence occurs. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. In Section 5.5.7, this handling is elaborated upon in a discussion provided by the SR-PSU team.

In the tables below, the operation, excavation and re-saturation period is excluded as it is short relative to the processes. Also the event of an earthquake is excluded as the event in itself is so short-term (even though it may provide new fracture surfaces).

Table 5-7. Direct influences of defined geosphere variables on the process "Reactions groundwater/rock matrix" and a short note of how the influences are handled in safety assessment SR-PSU. Abbreviations: T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.5.7)
Temperature in bedrock	Yes.	T/P/G	Constant temperature assumed in the hydrogeochemical modelling (Román-Ross et al. 2014).
Groundwater flow	No, but indirectly through: Groundwater composition.	T/P/G	–
Groundwater pressure	Yes.	T/P/G	Process neglected.
Gas phase flow	No, but indirectly through: Groundwater composition.	T/P/G	–
Repository geometry	No, but indirectly through: Groundwater flow and composition.	T/P/G	–
Fracture and pore geometry	No, but indirectly through the diffusion of solutes and water composition.	T/P/G	Pore geometry indirectly included in assessment through transport parameters (i.e. diffusivity) (**Radionuclide transport report**).
Rock stresses	No, but indirectly through: Fracture and pore geometry.	T/P/G	–
Matrix minerals	Yes.	T/P/G	Rock minerals are taken into account in assessment of evolution of groundwater composition (see Román-Ross et al. 2014).
Fracture minerals	No, but indirectly through: Groundwater composition.	T/P/G	–
Groundwater composition	Yes.	T/P/G	Groundwater composition included in assessment of evolution of groundwater composition (Román-Ross et al. 2014).
Gas composition	No, but indirectly through: Groundwater composition.	T/P/G	–
Structural and stray materials	No, but indirectly through: Groundwater composition.	T/P/G	–
Saturation	Yes.	T/P/G	Fully saturated conditions assumed.

Explanation of Table 5-7

Temperature in bedrock

The temperature influences the rates of reactions in the rock matrix. The influence of temperature on groundwater/rock reactions can be neglected since the impact is expected to be small in the expected temperature range.

Groundwater flow

The influence is indirect by affecting the groundwater composition.

Groundwater pressure

The groundwater pressure influences reaction rates. In the expected pressure range the influence is small and can be neglected.

Gas phase flow

The influence is indirect through influence on the groundwater composition. Dissolved gasses can diffuse into the rock matrix in the pore water and react with matrix minerals.

Repository geometry

The influence is indirect through influence on the groundwater composition and flow by short-circuiting hydraulically conductive fractures. This may change the groundwater composition.

Fracture and pore geometry

The fracture and pore geometry influence mineral surfaces accessible to reactions. The pore geometry also affects the diffusive transport of solutes from the fracture water into the rock matrix, and vice versa.

Rock stresses

The influence is indirect by influencing the pore geometry.

Matrix minerals

The rock minerals may react with solutes in the pore water or fracture water. This affects the pore water and fracture groundwater composition. For example, biotite in the rock matrix may affect the redox potential of the groundwater in the fractures. As a consequence the buffering capacity of the system to changes in redox potential of inflowing groundwater is affected by matrix minerals.

Fracture minerals

The influence is indirect as fracture minerals could function as a transport resistance for solutes diffusing in and out of the rock matrix. Thereby, both the pore water and groundwater composition may be affected.

Groundwater composition

The reactions that may occur between pore water and the rock matrix are dependent on the composition of the groundwater in the fractures through diffusion of solutes.

Gas composition

The influence is indirect by influencing the groundwater composition, through dissolution or degassing.

Structural and stray materials

The influence is indirect by groundwater compostions such as pH, microbial activity (cf. Section 5.7 and Section 5.8) in fractures, locally.

Saturation

Reactions between rock and porewater can only occur in water saturated portions of the rock matrix.

Explanation of Table 5-8

Temperature in bedrock

The temperature in the bedrock is influenced by production or consumption of heat during reactions. This contribution is negligible compared to heat conduction.

Groundwater flow

The rock matrix, in terms groundwater/rock matrix interactions, has very minor impact on the groundwater flow, by way of affecting the groundwater composition. This could affect the groundwater flow (through density driven flow) but in reality the groundwater/rock matrix interactions are too slow to have a real effect.

Table 5-8. Direct influences of the process "Reactions groundwater/rock matrix" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.5.7.)
Temperature in bedrock	Yes, but minor.	T/P/G	Influence neglected.
Groundwater flow	No, but indirectly through: Groundwater composition.	–	–
Groundwater pressure	No.	–	–
Gas phase flow	No. but indirectly through: Groundwater composition	T/P/G	–
Repository geometry	No.	–	–
Fracture and pore geometry	Yes.	T/P/G	Influence neglected.
Rock stresses	No, but indirectly through: Fracture and pore geometry.	T/P/G	–
Matrix minerals	Yes.	T/P/G	The fate of matrix minerals is not assessed in SR-PSU.
Fracture minerals	No, but indirectly through: Groundwater composition.	T/P/G	–
Groundwater composition	Yes.	T/P/G	Rock minerals are taken into account in the assessment of evolution of groundwater composition (Román-Ross et al. 2014).
Gas composition	No, but indirectly through: Groundwater composition.	T/P/G	–
Structural and stray materials	No.	–	–
Saturation	Yes.	T/P/G	Influence neglected.

Groundwater pressure

Any effect on groundwater pressure by groundwater/rock matrix interactions would be insignificant.

Gas phase flow

The influence is indirect via the pore water contents of dissolved reactive gases such as O_2 and CO_2, which subsequently may come out of solution. This contribution is negligible compared to gasses originating from the waste and engineered barriers.

Fracture and pore geometry

Weathering reactions may increase or decrease the porosity of the rock matrix.

Rock stresses

Precipitation in the microporous system of the rock matrix, filling and expanding previous void, is not though to create a force on the surrounding matrix minerals to such a degree that the overall rock stresses are affected.

Matrix minerals

The matrix minerals can be affected by weathering reactionsalterations and is most prominent close to the fracture walls. The chemically altered zone close to the fracture wall is usually called wall rock.

Fracture minerals

The effect is indirect through pore water chemistry and matrix diffusion; however, this is for many minerals a very slow process under low-temperature conditions.

Groundwater composition

The fracture groundwater composition is affected by mineral dissolution and precipitation, as well as by reactions with the rock matrix. However, for the Al-silicates in the rock matrix, the process is very slow under low-temperature conditions

The specifics of the rock mineral surfaces also affect the distribution of solutes in the pore water. The mineral surfaces are generally negatively charged at the host rock conditions; although the occurrence of minor amounts of positively charged mineral surfaces cannot be excluded. The negatively charged surfaces generally attract cations, which may sorb, and repels anions, resulting in so called anion exclusion. This is further discussed in Section 6.2.

Gas composition

The effect is indirect by changing the pore water contents of dissolved reactive gases such as O_2 and CO_2.

Saturation

Pore water–rock reactions do not result in the production of gaseous products which may locally affect the water saturation. The influence is considered negligible.

5.5.3 Boundary conditions

The large scale boundaries concerning the groundwater flow and composition are found at the host rock/ground surface system interface and at the host rock/engineered repository interface. In this way, the ground surface system as well as the engineered repository, influences the flow and composition of the groundwater in the fractures in the host rock. This groundwater will interact with the rock matrix, where the small-scale boundary condition is at the groundwater/rock matrix interface.

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 considered to be sufficient. Knowledge of the reaction kinetics is less satisfactory, which makes it difficult to establish what time spans need to be postulated to achieve equilibrium.

Modelling of oxygen consumption during intrusion of glacial waters was modelled in SR-Site (Sidborn et al. 2010). Other work done in Sweden and Finland is summarised in Alexander and Neall (2007).

5.5.5 Natural analogues/observations in nature

There are many examples from nature which underline the water–rock reaction sequence from the introduction of meteoric water at shallow depths, to the evolution of deeper groundwaters of increasing salinity, to finally the formation and existence of deep-seated brines. A review of natural analogues regarding oxygen consumption in the bedrock has been presented in Sidborn et al. (2010).

Water–rock reactions in crystalline rock environments have been addressed by numerous studies in Finland and Sweden (e.g. Blyth et al. 2000, Pitkänen et al. 2002, Négrel et al. 2003, Laaksoharju et al. 2008b, 2009, Drake et al. 2009, Sandström et al. 2010).

5.5.6 Time perspective

At very low water/rock ratios, the minerals in the rock matrix can be regarded as stable due to the slow kinetics of the reactions. Fluids introduced into the rock matrix by diffusion or along micro-fractures can induce fluid–rock reactions. The low temperatures prevailing in the rock at present make these reactions very slow.

Chemical reactions that influence the composition of the water occur in a timeframe of microseconds to hundreds of thousands of years. The prevailing chemical groundwater composition is the result of many different on-going reactions and mixing of different waters (Laaksoharju et al. 2008a).

5.5.7 Handling in safety assessment

In this section, the SR-PSU team describes how the process of reactions between groundwater and rock matrix is handled. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-7 and Table 5-8 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

During the excavation/operation phase, and also during the re-saturation of the host rock, when Baltic Sea waters are expected to flow in fractures in the vicinity of the tunnels, or in the excavation damaged zone, chemical reactions are predominantly expected to take place at the surfaces of fractures and only to a minor degree in the rock matrix. This period is not modelled in with respect to groundwater/rock matrix interactions.

Periods of the temperate climate domain

The process is not deemed to cause appreciable changes in rock matrix porosity or mineralogy for the whole time period during which the function of the repository must be considered. Therefore the fate of matrix minerals is not assessed in SR-PSU.

Concerning the groundwater composition, the principal minerals existing in the rock matrix are included in the hydrogeochemical modelling (Román-Ross et al. 2014, Auqué et al. 2013).

Periods of the periglacial climate domain

The process is not deemed to cause appreciable changes in rock matrix porosity or mineralogy. Accordingly, no such changes are modelled within periods of the periglacial climate domain. The principal rock matrix minerals are included in the hydrogeochemical modelling (Román-Ross et al. 2014).

Periods of the glacial climate domain

In the event of a glaciation at the SFR area, there will be periods of large groundwater inflow to the repository. During such circumstances groundwater/rock matrix interactions would do little to alter (or buffer) the groundwater composition. In any case groundwater/rock matrix interactions should be subordinate to groundwater interactions with cementitious materials in the repository. Accordingly, glacial melt water from the surface is assumed to penetrate down to repository depth practically unaffected by water–rock interactions.

Earthquakes

Fracturing of the rock due to earthquakes is not likely to have a significant effect on the hydrogeochemistry at repository depths, unless fracturing causes significant changes in the flow conditions, resulting in mixing of different groundwaters and fast transport paths from the surface system down to the repository. Mixing of groundwaters could lead to dissolution and/or precipitation processes between water and rock matrix. As there are already relatively fast transport paths between the surface system and the repository (as some vaults are intersected by fracture zones), the potential effect of earthquakes on groundwater composition is not modelled within SR-PSU.

Handling relative to geosphere variables

Temperature in bedrock

Although a bedrock temperature of 15°C is used in hydrogeochemical modelling (Román-Ross et al. 2014) and this is somewhat elevated relative to the site, the influence of temperature changes is neglected since the influence has little impact compared with other uncertainties.

Groundwater flow

There is no direct dependency between groundwater flow and water–rock interaction.

Groundwater pressure

The influence is neglected since it has negligible impact compared with other uncertainties.

Gas phase flow

In principle, gasses could dissolve and interact with the rock matrix as solutes. However, such an impact is not modelled in SR-PSU.

Repository geometry

There is no direct dependency between repository geometry and water–rock interaction.

Fracture and pore geometry

In principle, all groundwater/ rock matrix interactions are dependent on the solute transport properties of the rock matrix. For example, the redox buffering capacity of the rock would primarily need to be accessed via matrix diffusion of solutes, even though some contribution could come from the fracture/rock interface (cf. Sidborn et al. 2010).

The fracture and pore geometry could in principle be affected by groundwater/ rock matrix interactions. It is unlikely that minerals would dissolve to such a degree that the overall fracture and pore geometry would be altered. On the other hand, the geometry of the microporosity of the rock matrix could be changed by the precipitation of very small amounts of material.

Rock stresses

There is no significant dependency between rock stresses and water–rock interactions.

Matrix minerals

The matrix minerals of course affect the reactions between pore water and the rock matrix. The principal minerals existing in the rock matrix are included in the hydrogeochemical modelling (Román-Ross et al. 2014). Matrix minerals are especially important in terms of the redox capacity of the groundwater at repository depth.

Fracture minerals

Groundwater and fracture mineral interactions are described in Section 5.6. Fracture minerals may indirectly interact with rock matrix minerals through alteration caused by solute diffusion in the matrix pores, but this in not taken into account in SR-PSU modelling as justified by the low importance of such interactions.

Groundwater composition

The interaction between fracture groundwater and rock matrix minerals is considered in the modelling reported in Román-Ross et al. (2014).

Gas composition

In principle, gasses in a gas phase could dissolve and interact with the rock matrix as solutes. However, such an impact is not modelled in SR-PSU. This is justified as the amount of substance (e.g. CO_2) transported by a gas flow, available for precipitation, is very small.

Structural and stray minerals

Cementitious structural and stray materials (e.g. grouting) could contribute to a hyperalkaline groundwater plume that could interact with matrix minerals and hence affect them. In the SFR repository, such a contribution would be subordinate to the contribution from cementitious material in the rock vaults, and is not specifically accounted for.

Saturation

In SR-PSU, all groundwater/rock matrix interactions are assumed to proceed at fully water saturated conditions.

5.5.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Many different mineral alteration reactions influence the evolution of the groundwater chemistry. 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 SR-PSU time span of 100,000 years.

Model simplification uncertainties

In SR-PSU, the pore geometry and mineral composition of the rock matrix is assumed to be constant throughout the assessment time, as discussed in Auqué et al. (2013) and Román-Ross et al. (2014). In addition the rock matrix is assumed to be homogeneous and infinite. This can be seen as a modelling simplification although it is believed that this simplification has a negligible impact on the assessed radiological risk.

5.5.9 Adequacy of references supporting the handling in SR-Site

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

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 and mixing of groundwaters. Products from the dissolution reactions are either removed, and this promotes further dissolution, or new reactants are brought in contact with the solid phases. In addition to advection/mixing, other factors that may induce dissolution or precipitation of fracture infillings are diffusion, changes in temperature, pressure, pH, redox conditions and salt exclusion induced by freezing (e.g. Puigdomenech 2001, Sandström et al. 2009). Microbial activity can also have a significant influence on these processes. For example, sulphide may precipitate due to microbial reduction of sulphate in the groundwater, and calcite may dissolve/precipitate due to microbial production of carbon dioxide during decomposition of organic matter (see Section 5.7).

Under steady-state conditions, these processes are as a rule quite slow. In the case of transient processes, e.g. infiltration (inflow) of acidic 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.

Detailed fracture mineralogical studies of fracture minerals have been carried out on selected drill cores within the SFR site investigation. The data are presented in Sandström and Tullborg (2011) and Sandström et al. (2011, 2013).

Reactions between water and fracture-filling minerals give rise to conversion (alteration) of the mineral phases. At the ground surface, this phenomenon is called chemical weathering, and the mineral phases formed consist e.g. of different kinds of clay minerals and iron(oxy)hydroxides. Many bedrock fractures have experienced complex sequences of alterations and in many cases an evolution with repeated reactivation and dissolution/precipitation of fracture minerals. The sequence of different events of fracture mineral precipitation at Forsmark has been described by Sandström et al. (2009). Most fracture-filling minerals at Forsmark have originated under hydrothermal conditions (temperatures above 200°C) during the Precambrian (> 540 Ma) or from brine-type fluids at temperatures between 60 and 190°C during the Palaeozoic (> 250 Ma) (Sandström et al. 2009). Subsequently, minerals in water-conductive fractures have been subjected to alteration on several different occasions under low-temperature conditions.

Precipitated fracture minerals, such as calcite, pyrite, zeolites and iron oxides, make it possible to draw conclusions concerning the water chemistry that prevailed when the minerals were formed (Sandström and Tullborg 2009). By contrast, the opposite reaction, dissolution of fracture-filling minerals, is difficult to identify and quantify. Rapid transport of carbon dioxide-rich water can, for example, dissolve calcite in a flow path relatively rapidly, and subsequently cause precipitation of calcite on fracture surfaces further down the flow path when mixing with other types of water.

Human activities such as drilling may influence the groundwater composition by short-circuiting groundwaters with different hydrochemistry, as will the construction of a repository. This may to some extent cause changes in the fracture mineral population of the affected flow paths.

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 especially in clay minerals along with dissolution and precipitation reactions. As a result of these reactions, the water, regardless of whether it is fresh or saline, will have particular proportions of sodium and calcium. Infiltration of meteoric water with low pH promotes silicate weathering and subsequent release of sodium and calcium.

Influence on magnesium and potassium concentrations: The cations magnesium and potassium are common in groundwater and are specifically introduced to the bedrock aquifers during seawater intrusion, but their concentration is kept down by uptake by ion exchange (primarily on clays) and possibly also by some mineral formation reactions (e.g. clays and K-feldspar). This is clearly evident at sites where seawater has infiltrated the rock and the concentrations have fallen from originally high marine Mg/Cl and K/Cl ratios to lower ratios in the fracture groundwater (Laaksoharju et al. 2008b, 2009).

Influence on ^{14}C concentrations: Carbon-14 is quite mobile since it is transported in solution as weakly-sorbing anionic species such as HCO_3^- and CO_3^{2-} and as dissolved H_2CO_3 and CO_2 depending on the pH (Sheppard et al. 1998, Walke et al. 2009). Precipitation of calcite ($CaCO_3$) is an important process in the geosphere for removing ^{14}C from the groundwater. During precipitation of calcite, ^{14}C is somewhat enriched in the solid phase by fractionation although the extent of fractionation is small (Wigley 1976). Furthermore, retardation of ^{14}C can be promoted by isotopic exchange with calcite and sorption of ^{14}C onto calcite and goethite surfaces (Garnier 1985, Sheppard et al. 2006). Experimental data shows that carbon sorption generally is weak at near-neutral pH but can be strong at pH < 6 (Allard et al. 1981, Linklater et al. 2003, Baik et al. 2010). Dissolution of calcite has an isotopic dilution effect on the activity of ^{14}C in the groundwater (cf. Smellie et al. 2008).

The initially elevated pH near the SFR repository due to degradation of concrete and grout will promote elevated pH and possible calcite precipitation and thus, at least in this respect, may promote retardation of ^{14}C.

Influence on pH: At present at SFR, pH values between 7 and 8 have been measured in the bedrock water samples (Nilsson A-C et al. 2010). These measurements should not be affected by degradation of cementitious materials, as water flows towards SFR. In the absence of cementitious materials, of greatest importance for the pH in the infiltrating groundwater are reactions between carbon dioxide dissolved in the water and calcite in the rock's fracture system and overburden. The carbonate system quickly reaches a state of equilibrium and determines the water's pH, which will then be weakly alkaline (Stumm and Morgan 1981). Measured bicarbonate concentration at SFR repository depth varies from 60 to about 160 mg/L (Nilsson A-C et al. 2010).

Waters emanating from within the SFR repository will generally have an increased pH due to degradation of concrete and grout. This may give rise to a so-called hyperalkaline plume. The secondary minerals replacing silicate minerals at high pH are preferentiallycalcium silicate hydrates (CSH) (Savage 1998 in Smellie 1998).

The carbonate content of non-saline deep waters declines with increasing residence time. As a result of feldspar weathering which releases calcium, precipitation of calcite may further lower the carbonate concentration. However, the pH-buffering capacity of the dissolved carbonate in the groundwater, which determines the pH, is small in comparison with the buffering capacity in the minerals. The amount of calcite that coats the fracture surfaces is of greater importance for buffering against acidification than the carbonates in the aqueous phase. At lower pH, e.g. following carbonate depletion, feldspars have a large capacity to buffer against acidification (e.g. Nordstrom et al. 1992, Descourvières et al. 2010).

Calcite is a useful indicator of inflow of recently infiltrated groundwater since near-surface dissolution of calcite often is an indication of inflow of acidic groundwater as shown at Laxemar (Drake et al. 2009). Calcite occurs as fracture-filling mineral evidence in around 40–80 percent of the water-bearing fractures at SFR and no evidences for calcite dissolution in the upper parts of the bedrock have been found (Sandström and Tullborg 2011). During the Forsmark site investigation, quantitative mapping of fracture minerals in water-conducting fractures and near-by fractures was carried out (Löfgren and Sidborn 2010). No corresponding mapping has been carried out during the SFR site investigation. However, applying the data of the abundance of fracture minerals from the Forsmark site investigations of the SFR area is considered conservative in the sense that it minimises the risk for overestimating the pH-buffering and reducing capacities (Sandström et al. 2013). Fracture-coating calcite constitutes an effective buffer against infiltrating acidic groundwater. How acidification will affect the groundwater composition at repository level for the nuclear waste has been modelled and described in Wersin et al. (1994). Hence, it may be concluded that the capacity of the minerals in the rock at the Forsmark site is sufficient to buffer against any acidification that can reasonably be expected. The same assumption can be made for the more superficial SFR repository, especially considering the amounts of concrete present within the SFR repository. In addition, the till cover above SFR has a high content of calcite (Hedenström and Sohlenius 2008), and constitutes as a substantial buffer against penetration of acidic groundwater.

Influence on redox conditions; The redox buffering capacity lies in the amount of available iron(II)-bearing minerals in the fractures and in the rock matrix, which react rapidly. Iron(II)-bearing chlorite, clay minerals and pyrite are the most abundant fracture minerals with reducing capacity at SFR (Curtis et al. 2011, Sandström and Tullborg 2011, Sandström et al. 2013). The rock matrix, which will be accessed by diffusion, makes up, by far, the largest potential reducing capacity. This effect will become active where there are no reducing minerals in the fractures, or when originally present fracture minerals, have been exhausted.

Co-precipitation of radionuclides; Precipitation and dissolution reactions may affect radionuclide transport (see Sections 6.1 and 6.2). Small amounts of radionuclides may be retained 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, Curti 1999). However this process is not included in the safety analysis (radionuclide transport modelling).

5.6.2 Dependencies between process and geosphere variables

In this section, dependences are identified between the process "dissolution/precipitation of fracture-filling minerals" and defined geosphere variables that are commonly expected in fractured crystalline rock at the SFR site in Forsmark. Table 5-9 outlines how the process is influenced by the defined geosphere variables, while Table 5-10 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence occurs. The influence between the process and each geosphere variable is elaborated upon below.In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU (see Section 5.6.7).

In the tables below, the operation, excavation and re-saturation period is excluded as it is so short relative to the concerned processes. Also the event of an earthquake is excluded as the event in itself is so short-term (even though it may provide new fracture surfaces).

Explanation of Table 5-9

Temperature in bedrock

Reaction rates and solubilities are temperature dependent. However, changes in temperature may be neglected in the relative narrow temperature range expected for SFR, since they are considered to have little significance compared with other influences.

Groundwater flow

The groundwater flow influences indirectly through advection of solutes e.g through mixing, necessary to the precipitation and dissolution reactions.

Table 5-9. Direct influences of defined geosphere variables on the process "Dissolution/precipitation of fracture-filling minerals" and a short note of how the influences are handled in safety assessment SR-PSU. Abbreviations: T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.6.7)
Temperature in bedrock	Yes.	T/P/G	Neglected: Constant temperature is assumed.
Groundwater flow	No, but indirectly through: Groundwater composition.	T/P/G	–
Groundwater pressure	Yes.	T/P/G	Influence neglected.
Gas phase flow	No, but indirectly through: Groundwater composition.	T/P/G	–
Repository geometry	No, but indirectly through: Groundwater composition.	T/P/G	–
Fracture and pore geometry	No, but indirectly through groundwater flow and composition.	T/P/G	The possibility of major precipitation, significant for a fracture geometry and flow and associated with high pH plume, is examined. Precipitation/dissolution reactions are assumed to take place on fracture surfaces (Román-Ross et al. 2014).
Rock stresses	No.	T/P/G	–
Matrix minerals	No, but indirectly through: Groundwater composition.	T/P/G	–
Fracture minerals	Yes.	T/P/G	Fracture minerals are taken into account in assessment of evolution of groundwater composition (Román-Ross et al. 2014).
Groundwater composition	Yes.	T/P/G	Groundwater composition is taken into account in the assessment of groundwater evolution (Román-Ross et al. 2014).
Gas composition	No, but indirectly through: Groundwater composition.	T/P/G	–
Structural and stray materials	No, but indirectly through: Groundwater composition.	T/P/G	–
Saturation	Yes.	T/P/G	Fully saturated conditions are assumed.

Groundwater pressure

Changes in pressure can change the solubility of fracture minerals. However, the effect on reaction rates and solubilities can be neglected due to little impact.

Gas phase flow

The influence is indirect by providing nutrients that, upon dissolving in the groundwater, are available for microbes. This allows for microbially mediated reactions that change the stability of fracture minerals.

Repository geometry

The influence from the repository geometry is indirect via changes in flow through hydraulically active fracture zones that may become short-circuited, and subsequent changes in water composition.

Fracture and pore geometry

The fracture and pore geometry influences indirectly via changes in the flow that could influence changes in the groundwater composition. Furthermore, all precipitation/dissolution reactions of fracture filling minerals take place at the fracture surfaces.

Rock stresses

Rock stresses may influence the process through a chain of indirect dependencies. For the SFR host rock, during the 100,000 years of assessment time, such influences are likely insignificant.

Matrix minerals

Matrix minerals influence the process indirectly, through groundwater composition, by the release of ionic species that may be incorporated in fracture precipitation phases.

Fracture minerals

The nature of the fracture filling minerals of course affects the dissolution/precipitation of the fracture filling minerals. Existing fracture filling minerals aid further precipitation by aiding nucleation and growth of the same, or other, precipitating fracture phases. Existing minerals are also a source of dissolved solutes.

Groundwater composition

The groundwater composition in terms of degree of chemical saturation determines, together with kinetics and the presence of solid phases, whether there will be precipitation or dissolution, or if there is equilibrium. See overview/general description.

Gas composition

The influence is indirect via groundwater composition; e.g. methane may be a source of nutrients for microbially mediated reactions that could induce mineral precipitation.

Structural and stray materials

Structural and stray materials such as grouting influence the process indirectly by increasing the pH and altering the composition of the groundwater.

Saturation

The host rock where dissolution/precipitation occurs is assumed to be fully water saturated. In principle, precipitation may occur as the degree of water saturation decreases, upon evaporation. However, this is not applicable in the safety assessment.

Table 5-10. Direct influences of the process "dissolution/precipitation of fracture-filling minerals" on the defined geosphere variables, and a short note of how the influences are handled in safety assessment SR-PSU. Abbreviations: T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.6.7)
Temperature in bedrock	Yes.	T/P/G	Influence neglected.
Groundwater flow	No, but indirectly through: Fracture and pore geometry.	T/P/G	–
Groundwater pressure	No.	–	–
Gas phase flow	No, but indirectly through: Fracture and pore geometry.	T/P/G	–
Repository geometry	No.	–	–
Fracture and pore geometry	Yes.	T/P/G	The possibility of major precipitation significant for fracture geometry and flow, is not accounted for in the geosphere, in the SR-PSU assessment.
Rock stresses	No.	–	–
Matrix minerals	No, but indirectly through: Groundwater composition.	–	–
Fracture minerals	Yes.	T/P/G	Fracture mineral phases are included in the evaluation of groundwater evolution (Román-Ross et al. 2014).
Groundwater composition	Yes.	T/P/G	Fracture minerals are taken into account in the assessment of evolution of groundwater composition (Gimeno et al. 2008).
Gas composition	No, but indirectly through: Groundwater composition.	T/P/G	–
Structural and stray materials	No, but indirectly through: Groundwater composition.	–	–
Saturation	No.	–	–

Explanation of Table 5-10

Temperature in bedrock

Reactions can produce or consume heat. However, the effect on temperature in the bedrock is negligible.

Groundwater flow

The influence is indirect by potential changes in small-scale fracture geometry (e.g. aperture) and large-scale fracture connectivity.

Groundwater pressure

The groundwater pressure does not change to a significant degree from dissolution/precipitation reactions. In this statement it is implied that any gas formed in the reaction can easily be evacuated from the system.

Gas phase flow

The influence is indirect by changing the groundwater composition, which may give rise to degassing or dissolution of gaseous compounds.

Fracture and pore geometry

Due to the relatively rapid dissolution and precipitation reaction of calcite, the flow paths in the rock may to some extent be changed if the chemistry of the infiltrating groundwater is changed. Open fractures may be sealed and previously sealed fractures may be opened due to changes in water chemistry. In the natural case, only in the event of major climate changes could this effect possibly be significant. The presence of Palaeozoic and even Precambrian calcite at Forsmark indicates that major events of calcite dissolution are not common in the area (Sandström and Tullborg 2009). However, the presence of the SFR repository, with all its cementitious components, may create a high pH plume that may lead to precipitation of calcium silicate hydrates that impacts the fracture minerals to such a degree that the overall fracture geometry is affected.

Rock stresses

Precipitation of fracture minerals, filling and expanding previous void, is not thought to create a force on the surrounding rock to such a degree that the overall rock stresses are affected.

Matrix minerals

Dissolution/precipitation of fracture minerals modifies the content of solutes in the groundwater/pore water which may affect the dissolution/precipitation of matrix minerals.

Fracture minerals

Dissolution/precipitation of fracture minerals influences fracture minerals by definition.

Groundwater composition

Dissolution and precipitation of fracture filling minerals influence the groundwater composition.

The specifics of the fracture mineral surfaces also affect the distribution of solutes in the contacting water for example through ion-exchange or sorption. The mineral surfaces are generally negatively charged at the host rock conditions; although the occurrence of minor amounts of positively charged mineral surfaces cannot be excluded (e.g. calcite within a certain pH range). The negatively charged surfaces generally attract cations, which may sorb by one or another process, and repel anions, resulting in so called anion exclusion. This is further discussed in Sections 5.4 and 6.2.

Gas composition

Compounds in the gas phase may dissolve and thus affect the dissolution/precipitation of fracture minerals. As an example, precipitation of calcite influences the amount of CO_2 in a possible gas phase: $CO_2(g) + H_2O + Ca^{2+}(aq) = CaCO_3(s) + 2H^+$.

Structural and stray materials

Fracture minerals, through their impact on groundwater composition, may to some degree affect the degradation of structural and stray materials such as rock reinforcements.

Saturation

Dissolution/precipitation reactions should generally not affect the degree of water saturation. If gasses are formed in the reaction to such degree that a free-phase gas is formed (which is unlikely), such a gas is assumed to be easily evacuated in the fracture system (see Section 3.3).

5.6.3 Boundary conditions

The large scale boundaries concerning the groundwater flow and composition, intimately associated with dissolution and precipitation of fracture minerals, are found at the host rock/ground surface system interface and at the host rock/engineered repository interface. In this way, the ground surface system, as well as the engineered repository, influences the flow and composition of the groundwater in the host rock. This groundwater will interact with the fracture minerals, where the small-scale boundary condition is at the groundwater/fracture surface interface.

One may also speak about chemical boundary conditions, affecting the degree of chemical saturation in the groundwater as well as the nature of the fracture filling minerals formed. The redox potential and pH are generally important chemical boundary conditions, but for the specific dissolution/precipitation reaction there are specific chemical conditions that need to be fulfilled. Also the temperature range expected at depth limits the dissolution/precipitation reactions that may take place.

5.6.4 Model studies/experimental studies

Numerous experiments have been conducted to explore both the reaction kinetics (Malmström et al. 1995) and the redox capacity (Pirhonen and Pitkänen 1991) of iron-bearing minerals. Site specific information on fracture mineral is given in Drake and Tullborg (2009a) and Sandström et al. (2008).

5.6.5 Natural analogues/observations in nature

In the Poços de Caldas project, the effects of co-precipitation as a retention process were evaluated for analogues to radionuclides (Bruno et al. 1996). Since then, several of the international and domestic analogue and site characterisation studies have addressed the mechanisms of radionuclide (and other trace element) retention in fractures from different types of host rocks representing different hydrogeological/hydrogeochemical environments (Tullborg et al. 1999, Kaija et al. 2000, Smellie 2002, Byegård et al. 2008). A review of natural analogues with a focus on redox processes is presented in Sidborn et al. (2010).

Fracture minerals can also be used to verify the present groundwater chemistry and to yield information about past groundwater conditions (palaeohydrogeology). The minerals used in such studies are mostly calcites, as this is a common fracture mineral that can form under various conditions. By analysing its stable isotope composition (O and C), Sr isotope ratio and its trace element contents, information about formation conditions can be obtained (Bath et al. 2000, Tullborg et al. 2003, 2008, Drake and Tullborg 2009b, Sandström and Tullborg 2009).

Analyses of fracture calcites have also been used to support the presence of former microbial activity in the fractures (Pedersen et al. 1997, Tullborg et al. 1999, Drake and Tullborg 2009b, Sandström and Tullborg 2009).

Uranium contents and uranium natural decay series analyses on groundwater and fracture minerals can indicate redox conditions over a time span of 2 Ma. In the Forsmark site investigations, mobilisation as well as re-deposition of uranium in the upper 150 metres of the bedrock is indicated. This is ascribed to the transition from near-surface oxidising conditions to more stable reducing conditions at depth (Sandström et al. 2008).

Valuable knowledge concerning mineral reactions at high pH has been obtained from the hyperalkaline sources in Maqarin in Jordan (Smellie 1998, Pitty 2011). The silicate minerals are dissolved as a consequence of hydrolysis reactions, after which secondary reaction products are precipitated (calcium silicate hydrates, CSH). 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.

A quantitative example of the capacity of feldspar as a pH buffer was given in a study in Poços de Caldas, Brazil, where a superficial groundwater with a pH of 3 was changed to 6–7 by reaction with feldspar (Nordstrom et al. 1992, Chapman et al. 1993).

5.6.6 Time perspective

The dissolution and precipitation reactions in the fracture systems are fast in comparison with the weathering of the host rock primary minerals. These reactions are therefore of importance in a 100,000-year perspective. During the period when the repository is open fracture minerals may be influenced locally, but the process is of minor importance.

Due to isostatic rebound, the ground surface above SFR will rise above the sea level during the initial part of the assessment time (see the **Climate report**). This will change the groundwater situation by introducing meteoric water into the upper part of the bedrock. This could promote dissolution of e.g. calcite and pyrite and precipitation of iron (oxy)hydroxides. Upon further isostatic rebound, a significant part of the host rock may become uplifted above the sea level. This will influence the groundwater flow pattern around the repository. However, the repository will still be covered by 50–120 metres of bedrock and additional sediments.

5.6.7 Handling in the safety assessment SR-PSU

In this section, the SR-PSU team gives recommendations on how to handle the process of dissolution/precipitation of fracture-filling minerals. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-9 and 5-10 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/resaturation period

Dissolution/precipitation of fracture-filling minerals, and the impact on groundwater composition, is not modelled during this period. This is justified the hydraulic gradient is directed towards the repository. Accordingly, if water flows in rock volumes directly adjacent to the repository, it will flow towards the underground openings. Hence, the groundwater composition is expected to be undisturbed by foreign materials in the repository. During this short time period, and under natural groundwater conditions, dissolution and precipitation of fracture-filling mineral can be disregarded.

Periods of the temperate climate domain

During periods of the temperature climate domain, dissolution/precipitation of fracture minerals will influence the groundwater composition and function as a buffer regarding pH and redox conditions. Therefore, the principal fracture minerals existing in the host rock are included in hydrogeochemical modelling (Román-Ross et al. 2014). Also, the closely located site Forsmark (Laaksoharju et al. 2008b), have comparable groundwater/fracture mineral interactions as the SFR site and can be used to understand the hydrogeochemical evolution of the SFR host rock (Nilsson A-C et al. 2010, 2011).

Concerning aqueous radionuclide transport modelling, sorption on fracture mineral surfaces is not accounted for. In practice it is assumed that the flow paths are bounded by undisturbed rock matrix. This is assumed to be conservative as justified in Section 6.2.

Periglacial climate domain

As for the temperate period, the principal fracture minerals existing in the host rock are included in hydrogeochemical modelling (Román-Ross et al. 2014).

Glacial climate domain

No groundwater composition modelling is performed in the case of a glacial period within the assessment time period but a glacial groundwater type is proposed (Auqué et al. 2013). It is assumed that the glacial melt water reaches down to the repository vaults. In that sense, the repository is short-circuited and water/rock interactions are neglected.

Earthquakes

Fracturing of the rock due to earthquakes is not likely to have a significant effect on the hydrogeochemistry at repository depths, unless fracturing causes significant changes in the water-flow, resulting in mixing of different groundwaters or fast transport paths from the surface system down to the repository. Mixing of groundwaters would lead to dissolution or precipitation of fracture minerals along water-conductive fractures. As there are already relatively fast transport paths between the surface system and the repository (as some vaults are intersected by fracture zones), the potential effect of earthquakes on groundwater composition is not modelled within SR-PSU.

Handling relative to geosphere variables

Temperature in bedrock

A typical but constant temperature is assumed in hydrogeochemical modelling (Román-Ross et al. 2014), and the influence of changes in temperature is neglected since the influence has little impact compared with other influences.

Groundwater flow

The potential for fracture mineral precipitation to the degree that it significantly alters flow paths is not investigated in SR-PSU.

Groundwater pressure

The influence is neglected since it has little impact compared with other influences.

Gas phase flow

The overall effect of dissolution/precipitation of fracture minerals on gas phase flow should be very small compared to the effect of gas production in the repository. No detailed gas phase flow in the geosphere is modelled in SR-PSU. Accordingly, potential production and disappearance of a gas phase in the geosphere are neglected.

Repository geometry

There is no direct dependency between repository geometry and dissolution/precipitation of fracture-filling minerals.

Fracture and pore geometry

The potential for fracture mineral precipitation to the degree that it significantly alters flow paths is not investigated in SR-PSU. Except for the case of a high pH plume, the fracture geometry is assumed to be unaffected by dissolution and precipitation of the fracture minerals throughout the assessment. This is justified by the generally slow water/rock interactions.

Rock stresses

It is assumed that there is no significant dependency between groundwater flow and dissolution/precipitation of fracture minerals.

Matrix minerals

The matrix minerals are assumed to be unaffected by groundwater/fracture mineral interactions.

Fracture minerals

The fracture minerals are in themselves of little concern for the SR-PSU safety assessment. For example, their capacity for radionuclide retention is neglected in radionuclide transport modelling (see Section 6.1). Their influence on groundwater composition (see below) is of interest, together with their possible impact on groundwater flow.

Groundwater composition

The principal fracture minerals existing in the host rock are included in hydrogeochemical modelling (Román-Ross et al. 2014). Also, the closely located Forsmark site, has comparable groundwater/fracture mineral interactions as the SFR site and can be used to understand the hydrogeochemical evolution of the SFR host rock (cf. Laaksoharju et al. 2008b). The most important parameters that could be affected by groundwater interactions with fracture minerals are redox potential and pH.

Gas composition

The gas composition may be affected by groundwater/fracture mineral interactions (e.g. CO_2). In this manner any $^{14}CO_2$ could be significantly retarded if dissolved or even participating in precipitation reactions, compared to in the free gas phase. However, this is pessimistically neglected when handling gas phase radionuclide transport (see Section 6.3).

Structural and stray materials

The degradation of cementitious structural and stray materials may contribute to the high pH plume. However, this contribution is insignificant compared to that of cementitious materials in the waste and engineered barriers. Therefore, it specific contribution is neglected in SR-PSU.

Saturation

Fully water saturated conditions are assumed in the SFR host rock (except for the initial few years after repository closure in repository adjacent rock).

5.6.8 Handling of uncertainties

Uncertainties in mechanistic understanding

The dissolution and precipitation of minerals are 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 which may not be well represented in thermodynamic databases. 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 SFR

Only precipitation and dissolution of solid phases that are known to have fast kinetics at low temperatures are used in hydrogeochemical modelling, e.g. carbonates, amorphous silica, Fe(III) oxides, oxyhydroxides, sulphates and sulphides (see Román-Ross et al. 2014).

The thermodynamic properties control mineral solubilities, of which not all are well established for fracture-coating minerals that have formed at low temperatures. The amount of Fe(II) available in the fracture system is based on a limited data set and no qualitative mapping has been carried out within the SFR site investigations (Sandström et al. 2013).

5.6.9 Adequacy of references supporting the handling in SFR

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.7 Microbial processes

5.7.1 Overview/general description

Microorganisms are ubiquitous in the environment and comprise a vast number of different species. Different microbial species are able to metabolise a wide range of energy sources and use a range of terminal electron acceptors during respiration. These metabolic processes are important geochemically, as they enhance the rate of kinetically hindered but thermodynamically favourable reactions. Different species are also able to tolerate different geochemical conditions and microbial diversity is maintained through the ability to enter a dormant state with low metabolic activity when external conditions become unfavourable. Therefore, as the biogeochemical conditions of a system change, the microbial population can change in composition and/or size.

The different metabolic pathways utilised by different types of microorganisms are detailed in the **Barrier process report** and will not be described in detail here. However, to summarise, respiration yields the most energy during aerobic respiration, in which oxygen is reduced as the terminal electron acceptor. The energy yield during anaerobic respiration decreases as the following terminal electron acceptors are used: nitrate, manganese, iron and then sulphate. The relative energy yields mean that when oxygen is available, for example, aerobic species dominate. Additionally, some bacteria use fermentative metabolism, which avoids the need for a terminal electron acceptor, and others are autotrophic, i.e. able to synthesise their own organic nutrients from inorganic H_2 and CO_2. Since microbial processes alter the chemical form of each species they utilise, they affect the water composition and the biogeochemical conditions of the subsurface environment. The development of biofilms may also alter the properties of the rock surfaces. Microbial population diversity is affected by the chemical and redox conditions, thus the natural microbial community in the vicinity of SFR may also be affected in terms of composition and/or cell number by the materials released from SFR.

Microbial cell numbers in deep granitic systems tend to be low, due to the low availability of nutrients. The dissolved organic carbon (DOC) concentrations in the shallow groundwater (4–119 m) of Forsmark have been found to be 1.1–1.4 mg/L (Lindquist and Nilsson 2010), which are within the range expected for typical Swedish deep granitic groundwaters (Allard et al. 1991). Likewise, the bacterial numbers of 10^3–10^5 per mL determined by Haveman and Pedersen (2002) are similar to those found in the Fennoscandian Shield in general.

SFR represents an important potential source of nutrients, electron donors and electron acceptors to the surrounding geosphere. These include organic materials in the waste and in cement additives in the concrete structures and grout, and hydrogen from anaerobic metal corrosion. The amounts of cellulose and organic complexing agents that will be deposited in SFR have been re-assessed (Keith-Roach et al. 2014). The formation of ISA, the main cellulose alkaline degradation product, was then calculated over time and its solution phase concentration was calculated taking sorption to the available hydrated cement into account. The ISA and organic complexing agent concentrations provide an indication of the organic material that could be in solution. Although the DOC concentration would be expected to decrease during diffusion or advection from these repository parts into the geosphere, it is feasible that the organics released will enhance the amount of dissolved organic material in the geosphere close to the repository.

Since ISA is expected to comprise a significant amount of the DOC in SFR, the question of whether ISA is a useable energy source is of importance both in terms of microbial activity and the impact of ISA as a complexing agent (see Section 5.4). Current work shows that microorganisms cultured from a high pH lime workings are capable of degrading ISA under aerobic and nitrate- reducing conditions and, to a lesser extent, under Fe(III)-reducing conditions (Bassil et al. 2013) in experiments initiated at pH 10 (Lloyd J R 2013, personal communication). Additionally, microbial species have been isolated from a range of environments that can degrade ISA under alkaline aerobic and nitrate-reducing conditions (Grant et al. 2002). Considering microbial adaptability, ISA degradation may therefore be expected to occur in parts of the geosphere around SFR (Humphreys et al. 2010). However, it should also be noted that the rate of ISA degradation will depend on the microbial species present, their adaptation to ISA and other available energy sources and other growth-limiting factors, such as the availability of accessible terminal electron acceptors for energetically favourable respiration processes (e.g. Rizoulis et al. 2012). The low availability of Fe(III) species in an alkaline environment may therefore limit Fe(III)-reducing anaerobic respiration; this question is often circumvented in experiments by the use of a growth medium and equally may be overcome in the geosphere by the presence of complexing agents, including ISA. Finally, the free energy released through anaerobic respiration decreases with an increase in pH (Rizoulis et al. 2012) and this, combined with the lower energy yields associated with anaerobic respiration in general, may limit the microbial activity in parts of the geosphere.

Individual microbial processes are dependent on the removal of waste products, as well as an ongoing supply of nutrients. However, microorganisms are diverse and adaptable, and active microbial communities have been found in isolated, deep subsurface environments where it is possible that different species utilize the limited available energy sources in a coordinated manner (e.g. Kovacik et al. 2006). Low groundwater flow is a safety function of SFR (SKB 2008c) and will influence the viable microbial community structure. Equally, a plume with highly alkaline leachates emanating from the concrete structures and grout would be expected to limit the diversity and size of the microbial population (Pedersen et al. 2004).

Radionuclides can be affected by microorganisms in a number of ways. For redox-sensitive radionuclides, microbially-mediated changes in the redox conditions can have an important influence on the radionuclide solubility and sorption characteristics. Some bacterial species can even use certain radionuclides in respiration processes (Lloyd et al. 2002). Radionuclides are also known to interact with microbial cells and biofilm surfaces (Anderson et al. 2006a, b). Biofilms can therefore modify the radionuclide sorption properties of fracture minerals. Active microorganisms can also produce and release organic chelators to mobilise essential trace elements. These can also interact with radionuclides and increase radionuclide mobility (e.g. Kalinowski et al. 2004, 2006).

Overall, it is difficult to predict the size and structure of the microbial communities over time in parts of the geosphere that are expected to be chemically-impacted by the repository. Therefore, predicting the effects of these uncertain microbial communities on radionuclide transport is even more challenging.

5.7.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-11 outlines how the processes are influenced by other geosphere variables, while Table 5-12 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. The influence between the process and each geosphere variable is elaborated upon below. In Section 5.7.7, the handling for all time periods, climate domains, and events is elaborated upon in a discussion provided by the SR-PSU team.

Explanation of Table 5-11

Temperature in bedrock

Temperature has a fundamental control over the rate of microbial processes, including respiration, and microbial species have temperature ranges in which they can function. However, temperature variations are expected to be low at repository depth until the onset of glaciation, and are of lesser importance than other influences in this period.

Groundwater flow

Groundwater flow will only have an indirect effect on microbial processes, via groundwater composition. The supply of nutrients and removal of waste products will affect the rate of metabolic processes and the community structure.

Groundwater pressure

Groundwater pressure will only have an indirect effect on microbial processes, via groundwater composition. This is because some gases, such as H_2 and CO_2, are metabolised by microorganisms, and their dissolution in the water is dependent on the pressure.

Repository geometry

The repository geometry will only have an indirect effect on microbial processes, via groundwater composition. The repository geometry affects groundwater flow patterns and the cross area of the alkaline plume, which influence microbial viability.

Fracture and pore geometry

The fracture and pore geometry will affect microbial processes directly, since cavities smaller than ~0.2 µm are not accessible to microbes. However, this has negligible impact on the overall microbial activity in the rock.

Table 5-11. Direct influences of defined geosphere variables on the process "microbial processes" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.7.7)
Temperature in bedrock	Yes.	E/O/S	Not handled explicitly, although the ambient temperature is sufficient to allow the microbial respiration of oxygen introduced into the system.
		T	Not handled, temperature variations will be very low in this period. Overall effect of temperature is less important than other influences.
		P/G	Microbial activity is considered to be very low in this period due to the frozen water and the limited input of nutrients.
Groundwater flow	No, but indirectly through its influence on the groundwater composition.		
Groundwater pressure	No, but indirectly through its influence on the groundwater composition.	–	–
Gas phase flow	No.	–	–
Repository geometry	No, but indirectly through its influence on the groundwater composition.	–	–
Fracture and pore geometry	Yes.	All	Neglected as this is of negligible impact on the overall microbial activity in the rock.
Rock stresses	No.	–	–
Matrix minerals	No, but indirectly through the influence on groundwater composition.	–	–
Fracture minerals	Yes.	All	Neglected, variations in the fracture minerals are of minor importance to the overall microbial processes.
Groundwater composition	Yes.	All	Used as an indicator of potential bacterial growth.
Gas composition	No, but indirectly through the influence of gas dissolution on the groundwater composition.	–	–
Structural and stray materials	No. Additionally, indirect effects via groundwater composition are unlikely to be significant in comparison to the influence of the waste and barrier system.		
Saturation	Yes.	E/O/S T	Neglected as sufficient water will be present to support life.
		P/G	Frozen water is considered to prevent significant microbial growth

Matrix minerals

Matrix minerals will only have an indirect effect on microbial processes. Dissolution and precipitation of matrix minerals will affect the groundwater composition, which in turn will influence microbial processes.

Fracture minerals

Several microbial respiration processes depend on electron acceptors that are present in some fracture minerals, for example Mn(IV) and Fe(III). Sulphides can be used as an electron donor by sulphur-oxidising bacteria if oxygen enters the system. However, variations in the fracture minerals are of minor importance to the overall microbial processes.

Groundwater composition

The groundwater composition has a direct effect on microbial processes. The groundwater provides energy sources and terminal electron acceptors for microbial metabolism and biofilm development. Organic materials and hydrogen released from SFR may increase metabolic activity. The metabolic waste products released into the groundwater may influence the viable microbial community. A highly alkaline groundwater pH is expected to limit microbial activity.

Gas composition

Gas composition will only have an indirect effect on microbial processes, via groundwater composition. This is because some gases, such as H_2 and CO_2, are metabolised by microorganisms, and their dissolution in the water is dependent on the composition of the gas phase.

Saturation

As for all life forms, liquid water is a requirement for microbial activity.

Table 5-12. Influences of the process “Microbial processes” on defined geosphere variables, and a short indication of how this may be handled in safety assessment. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.7.7)
Temperature in bedrock	No.	–	–
Groundwater flow	No, but indirectly via the fracture and pore geometry and groundwater composition	All	–
Groundwater pressure	No.	–	–
Gas phase flow	No.	–	–
Repository geometry	No.		
Fracture and pore geometry	Yes.	–	Neglected, biofilms are included implicitly in the assessment of current groundwater flow.
Rock stresses	No.		
Matrix minerals	No.		
Fracture minerals	Yes.	All	Not handled explicitly, judged to have a low impact on overall minerology.
Groundwater composition	Yes.	All	Process not handled in detail, but included implicitly within the general variations and uncertainities in the groundwater composition.
Gas composition	No, but indirectly via water composition.	–	–
Structural and stray materials	Yes.	All	Process not handled in detail. Included within the overall assessment of the degradation of stray materials in different time periods.
Saturation	No.	–	–

Explanation of Table 5-12

Groundwater flow

Microbial processes will only have an indirect effect on the groundwater flow, via the effect of biofilms on the fracture and pore geometry. They will also affect groundwater flow indirectly via microbially-driven changes in the groundwater composition, as this influences the precipitation/dissolution of secondary minerals.

Fracture and pore geometry

Biofilm formation will affect the fracture and pore geometry. Also, there is an indirect affect via microbially-driven changes in the groundwater composition and precipitation/dissolution of fracture minerals.

Fracture minerals

Microorganisms can extract components from fracture minerals thereby contributing to their weathering. Biofilm development can alter the mineral surface.

Groundwater composition

Microbial processes will consume nutrients and release waste products, altering the groundwater composition, dissolved gas concentrations, Eh, and pH. Changes in water composition may drive dissolution and precipitation reactions.

Gas composition

Microbial processes will affect the gas composition via water composition, since gaseous metabolic products will be released in the dissolved form.

Structural and stray materials

Microbial processes will oxidise accessible organic carbon in stray materials and hydrogen from metal corrosion if electron acceptors are available in sufficient quantities.

5.7.3 Boundary conditions

The boundary conditions for microbial processes are the concentrations of energy sources, electron acceptors and donors, and other macro and micro nutrients for growth (e.g. phosphorus) in the geosphere. The concentrations within different parts of the geosphere are dependent on transport from the three main inputs:

- Organic material and oxygen from the surface biosphere.
- Organic carbon and hydrogen from the repository.
- Hydrogen and methane from deep, subsurface gas-generating areas (Apps and van de Kamp 1993).

However, microbial consumption rates are also important in considering the depth/distance influenced by each input. Finally, the pH of the plume from SFR is a further boundary condition, with low microbial activity anticipated in highly alkaline groundwater (Pedersen et al. 2004, Rizoulis et al. 2012).

5.7.4 Model studies/experimental studies

The influence of alkaline conditions on microbial activity is an important question when assessing microbial processes in the geosphere. Recent work has shown that a microbial community from a high pH lime workings site was able to metabolise electron donors using nitrate and iron(III) as terminal electron acceptors in the pH range 9–11 (Rizoulis et al. 2012). However, active metabolism was not observed at pH 12, and sulphate-reduction was not observed at any pH studied, even when excess sulphate was added. The use of insoluble (low bioavailablity) ferrihydrite and soluble Fe(III)-

citrate as the Fe(III) source demonstrated that the form and therefore availability of a given terminal electron acceptor is an important factor. Additonally, Gibbs free energy calculations showed that both the ferrihydrite/Fe^{2+} and SO_4^{2+}/H_2S redox couples were energetically unfavourable in the pH range studied. The authors discussed the potential importance of complexing agents present in ILWs which may increase the bioavailability of Fe(III). Other work with these microorganisms has shown that the presence of "electron shuttles" such as riboflavin increase ferrihydrite reduction (Williamson et al. 2013) and that they can degrade ISA under aerobic and nitrate reducing conditions, and to a lesser extent, Fe(III)-reducing conditions (Bassil et al. 2013). The ISA experiments were initially at pH 10 (Lloyd J R 2013, personal communication).

A large and diverse array of investigations and experiments has been conducted to increase the understanding of microbial processes in deep groundwater and repositories. For the Fennoscandian shield, these have been reviewed in Pedersen (2001, 2002). Sampling procedures have been developed and thoroughly tested as have underground facilities for model studies (e.g. Nielsen et al. 2006, Hallbeck and Pedersen 2008c). The first important parameter to analyse in repository environments is biomass. Three different methods have been developed and found to correlate. Microscopic counts and biochemical analysis of adenosine-tri-phosphate (ATP) agreed well (Eydal and Pedersen 2007). The determination of cultivable microorganisms and ATP also agreed well when analysed (Pedersen et al. 2008). All types of microorganisms indicated in SKB (2010e, Figure 5-2) have been found via cultivation (Hallbeck and Pedersen 2008c), including fungi (Ekendahl et al. 2003, Reitner et al. 2005). The influence of viruses on microbial processes has been identified as an important factor to include in model studies. In particular, they seem to have an important mitigation effect on sulphide production by sulphate-reducing bacteria (Kyle et al. 2008, Eydal et al. 2009).

Microbial biofilms were found to significantly influence the sorption of radionuclides on glass and rock surfaces (Anderson et al. 2006a, b). In addition, it has been demonstrated that microbial iron oxidising biofilms are strong sorbents for trace elements (Anderson and Pedersen 2003, Anderson et al. 2006c). Microorganisms from deep groundwater produce complexing agents that mobilise radionuclides (Johnsson et al. 2006, Essén et al. 2007). Such complexing agents may have a strong influence on radionuclide mobility. They can mobilise uranium (Kalinowski et al. 2004, 2006) and strongly bind curium (Moll et al. 2008a) and uranium (Moll et al. 2008b). Interactions between SRB and curium have also been identified (Moll et al. 2004). Finally, it has been found that microorganisms can sorb radionuclides on their cell surfaces (Pedersen and Albinsson 1991), thereby facilitating mobilisation.

Microbial consumption of oxygen in a repository after backfilling has been modelled (Yang et al. 2007). It was found that presence of oxygen-reducing microorganisms decreased the time to consume all oxygen dramatically from several hundreds of years to a few weeks. A model to analyse microbial and geochemical reactive transport in porous media was successfully applied on field experiment data from an underground hard rock environment (Yang et al. 2008). Microbial metabolic processes have been included in transport models (Molinero et al. 2004) of a redox zone experiment (Banwart et al. 1994). The modelling supported previous conclusions on the importance of microbial processes in the reduction of oxygen with organic carbon (Banwart et al. 1996). The challenges and successes in modelling microbial processes for performance assessment have been reviewed by Humphreys et al. (2010).

5.7.5 Natural analogues/observations in nature

Analysis of the microbial community in the Forsmark area has focused on depths relevant to the spent fuel repository (e.g. Hallbeck and Pedersen 2012). Hallbeck and Pedersen (2012) assessed the microbial populations in a Forsmark borehole via the total cell number and ATP analysis, and examined species diversity using a variety of culture media. They found that the microbial populations in the Forsmark groundwater (112–978 m below sea level) were not correlated with depth, and contained nitrate-, iron-, manganese- and sulphate-reducing bacteria, as well as autotrophic acetogens, heterotrophic acetogens, autotrophic methanogens and heterotrophic methanogens. The total numbers ranged between $7 \cdot 10^3$–$5 \cdot 10^5$ cells/mL, and the ATP data generally correlated with the numbers of cells.

The alkaline springs of Maqarin have been thoroughly investigated for microbial activity (e.g. West et al. 1995, Pedersen et al. 2004). The results demonstrated that microorganisms from the hyperalkaline 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.

5.7.6 Time perspective

Significant microbial activity can be expected during the operation and closure phases of the repository, when significant oxygen will be available. During this period, organic material found at or near the repository will include grout cement additives, hydraulic oil spillage, pollen introduced with ventilation air, etc. These may be used as nutrients for microbial processes. However, grout, shotcrete and concrete elements will create zones of increased groundwater pH, which would be expected to reduce microbial activity significantly. After closure, microbial activity will continue at a rate controlled by the pH, reducing the available organic nutrients from the structural and stray materials. The groundwater chemistry will also influence the microbial processes taking place, for example, saline water contains elevated sulphate, enhancing the extent of microbial sulphate reduction once Fe(III) is reduced.

Changes in groundwater flow and chemistry induced by climate-related changes, e.g. by shoreline displacement, permafrost and ice sheets will affect the microbial activities in the geosphere. During periods of permafrost, the supply of nutrients will stop and water will be frozen. When the ice melts, the input of organic matter from the surface with recharge waters is also expected to be low, therefore microbial processes will be limited to those supported by dissolved methane and hydrogen production at depth and nutrient inputs from SFR.

5.7.7 Handling in the safety assessment

Anaerobic conditions induced by microbial activities from closure up to the post-glaciation period are considered in the safety assessment. The impact of microbial processes that increase the pH by generating CO_2 is also assessed (SKB 2008c). However, the generally low groundwater flow rates, the high pH in the plume from SFR and the relatively low microbial numbers/activity at depth, mean that the community is not expected to grow extensively. Therefore changes in the community are not assessed in detail over time and space. Additionally, the complexing agents arising from the waste and cement additives are expected to be much more abundant than organic complexing agents generated by microbial processes. Finally, the large uncertainties in the predicted climate evolution and the rate of SFR degradation, and the complexity of the microbial community response to these changes, would introduce unreasonable uncertainties in assessing this response and the resultant influence on radionuclide transport over time.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

The microbial community may be stimulated by organic stray materials and input of oxygen in the open repository period. As the repository is closed and resaturated, oxygen will be consumed and conditions will become reducing. Microbial activity will be limited in areas affected by high pH leachate from concrete components of SFR.

Periods of the temperate climate domain

The extent and type of microbial activity will be controlled by the pH of the plume, while outside the plume, any remaining stray organic material would be expected to be consumed more rapidly. Organic materials may be released from SFR, and these may stimulate the microbial population, depending on the flow and pH conditions.

Periods of the periglacial and glacial climate domains

Permafrost and glaciation will produce conditions that are unfavourable for most microbial activity. However, microorganisms can survive a permafrost, and possibly glaciation, and become active again as temperatures rise (SKB 2008c). Post-glaciation melt water will introduce water with a relatively low organic concentration. Although certain bacteria thrive in ice, microbial processes are expected to be relatively low in this period. There is the possibility that the combination of low microbial activity and elevated oxygen input result in oxidising conditions at repository depth (SKB 2008c).

Earthquakes

Although earthquakes are likely to affect microbial processes indirectly, they will not have a direct influence.

Handling relative to geosphere variables

Microbial processes are handled specifically in terms of the groundwater composition, as this affects the extent of growth and diversity. Indirectly, the groundwater flow is also an important variable as this affects the supply of nutrients and removal of waste products.

The microbial community is considered to maintain anaerobic conditions in the geosphere throughout the temperate period, and the effect of microbially enhanced carbonate concentrations is assessed.

5.7.8 Handling of uncertainties

Uncertainties in mechanistic understanding

The mechanisms of microbial processes are generally well known. However, there are large uncertainties when predicting microbial community structures and their response to the changes induced by SFR over the timescales of interest.

Model simplification uncertainties

Not applicable, since microbial processes will not be modelled.

5.7.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.8 Degradation of grout

5.8.1 Overview/general description

This section describes the degradation of the grout that is injected into rock fractures to reduce groundwater flow (during repository operation) and used to secure rock bolts. Degradation of the grout may influence the pH of its pore waters, which may diffuse into the surrounding groundwaters, and thus contribute to alkaline conditions at the repository vicinity. The impact of the plume of alkaline water on reactions in the groundwater/rock matrix and dissolution precipitation reactions of fracture-filling materials are discussed in Sections 5.5 and 5.6, respectively.

In many aspects the chemical processes in the degradation of grout are similar to those occurring in the concrete barriers, concrete packaging and cement waste matrices at SFR. Essential parts of the process are therefore presented in the **Barrier process report** and the **Waste process report** for SFR and also in the "Buffer, backfill and closure process report" for the safety assessment SR-Site (SKB 2010a). The grouting material comprises a small proportion of the total concrete and cement in SFR and therefore is expected to make only a small contribution to the overall effect of cement leachates on the geosphere.

Composition of grout

The injection grout is prepared by mixing unhydrated cement clinker minerals, with water. Typical unhydrated cement clinker minerals[8] and components are:

- Tricalcium silicate (Ca_3SiO_5), C_3S *(cement industry notation).*
- Dicalcium silicate (Ca_2SiO_4), C_2S.
- Tricalcium aluminate ($Ca_3Al_2O_6$), C_3A.
- Tetracalcium aluminate ferrite ($4\ CaO \cdot Al_2O_3 \cdot Fe_2O_3$), C_4AF.
- Calcium sulphate ($CaSO_4 \cdot 2H_2O$, "gypsum").
- Alkali hydroxides (e.g CaO), $N + K$.

Different additives can be used, e.g. to improve flow properties and workability of the freshly mixed grout slurry.

Cement hydration processes

Unhydrated cement clinker minerals react vigorously with water. These hydration reactions produce new (hydrated) solid compounds that give the grout its mechanical strength. The main binding phases of hydrated cement are calcium silicate hydrates (CSH) and calcium hydroxide (CH). In addition, two complex calcium sulpho ferri-aluminates[9], known as AF_t and AF_m, are major hydration products from reactions involving calcium aluminate, calcium alumino-ferrite and calcium sulphate.

Degradation of grout

Grout degradation may occur as a result of dissolution, precipitation and recrystallisation reactions, driven by interactions with groundwater and/or effluent from the SFR barriers. Concentration gradients between the grout porewater and the dilute groundwater at the rock interface will induce diffusive mass transport (of mainly Na^+, K^+, Ca^{2+} and OH^- ions) out from the porous grout (see Section 5.3).

Cement degradation is often described in three stages, as follows:
During stage I of cement degradation, the pore water will be dominated by the leaching of alkali metal (K^+, Na^+) hydroxides, producing highly alkaline conditions with a pH of about 13. Alkali metal hydroxides are generally soluble but chemical interactions with the solid phases retard their leaching from concrete (Lagerblad and Trägårdh 1994). Leaching of alkali metal hydroxides ions therefore decreases gradually, rather than in a stepwise manner.

During Stage II of cement degradation, the pH decreases sufficiently to enhance the solubility of calcium hydroxide (portlandite) in the cement. Equilibrium with portlandite buffers the porewater pH to 12.5.

During Stage III, incongruent dissolution of the CSH-gel takes place. This is accompanied by a gradually lowering of the pH down to about 10 (SKB 2008c).

The degradation of cement clinker minerals is described in further detail in the **Barrier process report** (see Section 5.4.6).

The dissolution of CSH is accompanied by the leaching of other minerals in the cement. AF_m dissolution releases $Al(OH)_4^-$, which will also diffuse out and could induce precipitation of secondary AF_m. However, groundwater components can influence the minerals precipitated, for example, ettringite forms in the presence of excess sulphate, and Friedelsalts (i.e. calcium-aluminium chlorides) form in the presence of chloride. Additionally, a combined attack by sulphate and carbonate at low temperature

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[8] Cement chemists' notation for the clinker components:

$C = CaO, S = SiO_2, A = Al_2O_3, F = Fe_2O_3, H = H_2O, C\hat{s}H_2 = CaSO_4 \cdot 2H_2O, N = Na_2O, K = K_2O$

[9] $AF_t = C_6(A,F)X_3H_y$ and $AF_m = C_4(A,F)XH_y$, where $X = CaSO_4$; $y = 32$ for ettringite and $y = 12$ for monosulphate.

may lead to precipitation of thaumasite ($Ca_3Si(OH)_6(SO_4)(CO_3)\cdot 12H_2O$) by reaction with AF_m/AF_t phases where silica from CSH-gel has replaced aluminate.

Waste components such as sulphate are expected to react with the conditioning cement or concrete barrier minerals before reaching the grout (SKB 2008c). These secondary minerals can enhance grout degradation due to their large molar volumes and crystalline morphologies. Therefore, unless sufficient pore volume is available to accommodate the mineral formed, formation could result in cracking and mechanical deterioration of the grout (Höglund 2001, Lagerblad 2001).

If the external groundwater contains dissolved carbon dioxide, precipitation of calcite might occur. In a modelling study, this has been found to reduce the degradation rate by sealing the pore network on the exposed surface of cement (Pfingsten 2001). A study by 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. Brucite may also be prone to precipitation at the grout–groundwater interface, due to its low solubility at high pH (Lagerblad 2001).

Organic chemicals are used as cement additives, including lignosulphonate-based plasticisers (used to increase flow properties and workability of the fresh concrete mix before hardening) and retarders that may include sugar, sucrose, sodium gluconate, glucose, citric acid, and tartaric acid (used to slow down the early hydration). Concrete additives are not known to cause degradation of the hardened concrete, and macromolecular additives tend to be strongly sorbed to the concrete minerals (Hakanen and Ervanne 2006). The chemical stability of organic concrete additives is further described in Section 3.5.6 in the **Waste process report**.

Conditions for processes to occur

The rate and extent of dissolution and precipitation processes in the grout is influenced by:

- The rate of advective water transport carrying dissolved species (see Section 5.2).
- The rate of diffusive transport of dissolved species (see Section 5.3).
- The composition of the grout including the assembly of hydrated cement clinker minerals.
- Any changes in the chemical composition of the grout induced by chemical reactions with surrounding rock/groundwater. This may in turn influence the microstructure of the concrete which would affect its transport properties.
- The composition of the pore water. This is in turn determined by local thermodynamic equilibria between the pore water and the solid hydrated cement minerals.
- Kinetic factors causing metastable equilibria, steady-state conditions, or slow establishment of equilibria.
- The composition of the groundwater and the pore water composition from the barriers in SFR.

5.8.2 Dependencies between process and geosphere variables

In this section, dependences between the process “Degradation of grout” and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-13 outlines how the process is influenced by other geosphere variables, while Table 5-14 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence occurs. The handling in the safety assessment SR-PSU is indicated in the rightmost column in the table. The influence between the process and each geosphere variable is elaborated upon below. In Section 5.8.7, the handling for all time periods, climate domains, and events is elaborated upon in a discussion provided by the SR-PSU team.

Table 5-13. Direct influences of defined geosphere variables on the process "Grout degradation" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.8.7)
Temperature in bedrock	Yes.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Groundwater flow	Yes.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Groundwater pressure	Yes.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Gas phase flow	Yes.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Repository geometry	No direct influence.		
Fracture and pore geometry	No, but indirectly via structural and stray materials.		
Rock stresses	Yes.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Matrix minerals	No, but indirectly via dissolution and groundwater composition.		
Fracture minerals	No, but indirectly via dissolution and groundwater composition.		
Groundwater composition	Yes.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Gas composition	No, but indirectly via the groundwater composition.		
Structural and stray materials	Yes, the amount and composition of the grout influences its degradation.	All	The influence is not handled in the safety assessment based on negligible consequences on performance and safety. Grout performance is not associated with any defined safety function of the geosphere.
Saturation	Yes.	T/P/G	The repository is assumed to be saturated instantaneously at closure, including the grout.

Explanation of Table 5-13

Temperature in bedrock

Temperature affects thermodynamic constants and therefore the chemical reactions that take place during grout degradation.

Groundwater flow

High groundwater flow could induce mechanical erosion of the grout. Additionally, the groundwater flow rate has an indirect influence on grout degradation due to its influence on the exchange of water that has equilibrated with the grout (see groundwater composition).

Groundwater pressure

Groundwater pressure can affect chemical reactions, although it only has a minor influence. Homogeneous hydrostatic pressure after the repository has re-saturated should not affect the mechanical integrity of the grout.

Gas phase flow

Large-scale gas flow may affect the mechanical stability of the grout, but this is considered to be of negligible importance.

Repository geometry

Indirectly, the geometry of the repository may influence the volume of grout required. The amount of grout is however included in the definition of the geosphere variable Structural and stray materials.

Fracture and pore geometry

The fracture and pore geometry has an indirect influence on grout degradation via the groundwater composition in the grout pore water which depends on diffusive and advective transport paths for dissolved components. Since the size of a fracture will determine the amount of grout present, it also has an indirect influence on grout degradation via the variable Structure and stray materials which includes the amount and composition of grout.

Rock stresses

The relaxation of rock stresses (e.g. through rock fall-out) and tectonic movement may cause cracking of the grout. This is not addressed specifically as the influence on injection grout is of low consequence on performance and safety.

Matrix minerals

The matrix minerals affect grout degradation processes indirectly as their dissolution reactions influence the groundwater composition.

Fracture minerals

The fracture minerals affect grout degradation processes indirectly as their precipitation and dissolution reactions influence the groundwater composition.

Groundwater composition

The groundwater composition will affect the type and extent of dissolution, precipitation and recrystallisation reactions that occur in the grout.

Gas composition

The gas composition will affect grout degradation processes indirectly via the groundwater composition, since the gas composition will be in equilibrium with the dissolved gases. Carbon dioxide is of particular importance, as it could lead to acidic dissolution of alkaline minerals, and/or calcite precipitation and the associated clogging of pores.

Structural and stray materials

Grout is regarded as a stray material in the geosphere, thus the type and amount of grout will influence its own degradation.

Saturation

The level of saturation will affect the rate at which the grout will be leached. A higher degree of saturation increases the leaching of cement components and thus accelerates grout degradation.

Table 5-14. Influences of the process "Grout degradation" on defined geosphere variables, and a short indication of how this may be handled in safety assessment. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.8.7)
Temperature in bedrock	Yes.	All	Not handled specifically as grout degradation involves negligible heat generation/loss.
Groundwater flow	Yes.	All	Not handled specifically. In the safety assessment, any flow limiting effect of grout is pessimistically neglected, at all times. See Section 3.2 on groundwater flow.
Groundwater pressure	Yes.	All	Not handled specifically. In the safety assessment, any flow limiting effect of grout is pessimistically neglected, at all times. See Section 3.2 on groundwater flow.
Gas phase flow	Yes.	All	Not handled specifically. The permeability of the grout is assumed to be sufficient to allow gas transport into the geosphere.
Repository geometry	No direct influence.		
Fracture and pore geometry	Yes, as degradation of grout progresses the porosity of the grouted fractures increases. Also indirectly via the influence of grout degradation on groundwater composition and dissolution/precipitation reactions.		Not handled specifically. In the safety assessment, any pore constraining effect of grout is pessimistically neglected, at all times. The grout is not envisaged to have any safety function in the safety assessment and its expected structural degradation is therefore not handled in the safety assessment.
Rock stresses	Yes.	All	Various aspects of mechanical processes are handled in Chapter 4. The stress contribution from grout degradation is however neglected and not handled specifically in the safety assessment.
Matrix minerals	No, but indirectly via changes in the groundwater composition, matrix diffusion, and dissolution/precipitation reactions.		See variable; Groundwater composition.
Fracture minerals	No, but indirectly via changes in the groundwater composition and dissolution/precipitation reactions.		See variable; Groundwater composition.
Groundwater composition	Yes.	All	Not handled specifically for grout.The volume of grout is relatively small compared to other cementitious materials in the SFR barriers and waste packages. Its overall contribution to the composition of SFR leachates into the geosphere is therefore neglected.
Gas composition	No direct influence. Any indirect gas generation or consumption as a consequence of grout degradation is negligible.		
Structural and stray materials	Yes, the degradation of grout will influence the amount and composition of the grout.	All	Not handled specifically. The grout is not envisaged to have any safety function and its expected structural degradation is therefore not handled in the safety assessment.
Saturation	No direct influence.		

Explanation of Table 5-14

Temperature in bedrock

Exothermic/endothermic chemical reactions can influence the ambient temperature. However, grout degradation involves negligible heat generation/loss.

Groundwater flow

As the grout degrades, its hydraulic properties will change and affect groundwater flow and consequently the groundwater pressure through the rock fractures.

Groundwater pressure

As the grout degrades, its hydraulic properties will change and affect groundwater flow and consequently the groundwater pressure through the rock fractures.

Gas phase flow

As grout degrades and cracks it may become more permeable and allow increased gas phase transport in the geosphere.

Repository geometry

No direct influence identified.

Fracture and pore geometry

As grout in the fractures degrades, the porosity of the grouted fractures will increase. Grout degradation may also influence dissolution/precipitation of minerals indirectly via changes in groundwater composition. This indirect influence may affect the fracture and pore geometry.

Rock stresses

As the grout degrades, the rock will be less supported (e.g. its function to secure rock bolts will be lost) which may affect the rock stresses (see Chapter 4 for the handling of various aspects of mechanical stresses). The stress contribution from grout degradation is restricted to the immediate vicinity of excavated rock volumes and is neglected in the safety assessment.

Matrix minerals

Grout degradation may induce dissolution/precipitation of minerals in the rock matrix indirectly via changes in groundwater composition and matrix diffusion.

Fracture minerals

Grout degradation will influence the groundwater composition, and thus may induce dissolution/precipitation of fracture minerals indirectly.

Groundwater composition

Grout degradation will affect the groundwater composition via dissolution, precipitation and recrystallisation reactions. The influence on the groundwater composition is however small compared to the influence of other more abundant sources of cement leachates (from the SFR waste packages and barriers). The contribution from injection grout is therefore neglected in the safety assessment.

Gas composition

No direct influence identified. Any indirect gas generation or consumption as a consequence of grout degradation is negligible.

Structural and stray materials

The degradation of grout will affect its own properties (amount and composition) as a stray material.

5.8.3 Boundary conditions

The boundary conditions for grout degradation are the groundwater and rock matrix porewater composition and the composition of the water entering from the waste and repository barriers. The water composition will determine the type and extent of reactions for the grout-water system, and the groundwater flow rate will then influence the overall rate of grout degradation.

Tectonic movement is also a boundary condition as this can expose previously undisturbed parts of the grout to groundwater (discussed in e.g. Sidborn et al. 2014).

5.8.4 Model studies/experimental studies

There have been a large number of studies investigating concrete degradation that are discussed in the **Barrier process report** (Section 5.4.6). These studies are also of relevance for the degradation of grout. Complex 2D- and 3D-geometries have recently been considered in mechanistic models of the degradation of concrete barriers in SFR (Höglund 2014) and in models of the development of an alkaline plume extending from grouted fractures in the vicinity of the ramp and shafts of the spent fuel repository at Forsmark (Sidborn et al. 2014).

5.8.5 Natural analogues/observations in nature

In the **Barrier process report** (Section 5.4.5) some natural analogue studies of alkaline cements are discussed. These are also of relevance for the degradation of grout.

5.8.6 Time perspective

The chemical degradation of the grout will produce an alkaline porewater over a significant part of the first temperate post closure period. The longevity of the grout will depend on the groundwater composition and the water flow rate around or through the grout. This means that the degradation of grout in the vicinity of a given vault will vary according to its position with respect to other concrete components, the direction of groundwater flow, and the extent of fractures and flow paths intersecting the grouted fractures in the rock.

The influence of grout degradation on the mechanical processes at the surface of the rock vault is discussed in Chapter 4. Grout is expected to have lost its load bearing capacity completely after about 200–250 years (SKB 2008c).

5.8.7 Handling in the safety assessment

Handling relative to time periods, climate domains, and events

Grout degradation is not specifically handled in SR-PSU. In the safety assessment, any flow limiting effect of grout is pessimistically neglected, at all times.

Handling relative to geosphere variables

Grout degradation and its influence on defined geosphere variables, is not specifically handled in SR-PSU. Any flow limiting effect of grout is pessimistically neglected in the safety assessment, at all times. Concrete degradation in SFR is handled specifically when assessing geosphere retention parameters (K_d) qualitatively in terms of effects on groundwater composition (Crawford 2013). The groundwater composition affects the dissolution, precipitation and recrystallisation reactions that take place in the concrete, and the reactions in turn affect the groundwater composition. Indirectly, the groundwater flow is also an important variable as this affects the rate at which degradation progresses and the flux of alkaline constituents from SFR into the geosphere. The groundwater flow through the repository vaults is modelled in conjunction with concrete degradation (Höglund 2014).

5.8.8 Handling of uncertainties

Uncertainties in mechanistic understanding

A major uncertainty is related to the complex solubility behaviour of CSH-phases, which has been represented by successively more complex modelling approaches in studies of cement degradation. This is discussed in Sidborn et al. (2014).

Uncertainties also concern the fate and properties of different calciumsulpho-aluminates, calcium-sulpho-ferrites (AF_m and AF_t), as well as similar calciumalumino- and calciumferrite- mineral phases formed by reactions with chloride and carbonate. Of particular interest here are the volume changes of the solid phases accompanying these reactions, which could result in clogging of fractures and pores in the rock matrix, and the potential precipitation/recrystallisation of expanding minerals causing fractures in grout and concrete. The mechanical pressures exerted by such mineral reactions are less well established and require further study and so far they are handled by conservative assumptions in the SR-PSU.

Other uncertainties are associated with the long-term evolution of the pore network and the diffusivity in the hydrated cement within the grout. The diffusivity depends strongly on the porosity values, and the coupling between the dissolution processes and the resulting micro-structural changes are not fully understood.

Model simplification uncertainties

Injection grout is not explicitly included as a separate component in SR-PSU, and thus is not handled in the concrete degradation models used within the safety assessment (e.g. Höglund 2014). This may be considered a model simplification. For simplifications regarding the process of concrete degradation, see the **Barrier process report** (Section 5.4.6).

5.8.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.9 Colloidal processes

5.9.1 Overview/general description

The term colloidal refers to a state of subdivision, in which molecules or polymolecular particles dispersed in a medium have at least one dimension between 1 nm and 1 μm (IUPAC 2011), and colloids can be inorganic or organic in nature. They tend to form through physical erosion or chemical precipitation processes. Their small size is important for two reasons: 1) colloids can be transported through many fractured or porous media, and 2) colloids have very high surface area to mass ratios. The high surface area to mass ratio gives the colloidal form of a material a much higher sorption capacity per unit mass than the bulk material. Therefore, relatively low concentrations of colloids can compete effectively with the solid phase for contaminant sorption. The impact of this process on contaminant transport depends on whether sorption is reversible or effectively irreversible over time scales associated with groundwater transport (see e.g. Alexander et al. 2011). Effectively irreversible sorption can therefore be required for colloids to have a significant impact on contaminant transport in slow flow regimes with relatively low colloid concentrations, see e.g. the studies by Vilks et al. (1991a, b) where the colloid concentration was < 1 mg/L.

The potential sources of colloids in the geosphere surrounding SFR include the following:

- Natural inorganic groundwater colloids include metal oxides, silica, carbonate, sulphide and clay minerals (van Loon and Duffy 2000). Colloids have been characterised in the vicinity of SFR but not in detail at the relevant depth; colloids in related environments are discussed in Section 5.9.5. Natural colloids are generated from the erosion of solid matrices or chemical reactions, and colloid concentrations are sensitive to changes in groundwater flow or chemistry.
- Organic colloids including humic and fulvic acids, highly branched macromolecules or aggregated smaller units with a capacity for reversible and effectively irreversible binding of radionuclides.
- Colloids from SFR wastes; the **Waste process report** and the **Barrier process report** suggest that most colloids, including cement colloids, will be unstable (see below) during the period of repository barrier function, however, there is less evidence for bitumen colloid instability. Any stable colloids may also be transported out of BLA and BRT, which have no engineered barriers and no safety function for restricted flow. Radionuclide intrinsic colloids are unlikely to form in any significant amounts in SFR due to the relatively low concentrations of radionuclides.

- Colloids from the bentonite in the Silo; the **Barrier process report** suggests that these colloids will be unstable (see below) during the period of repository barrier function.
- Microbial cells fall into the colloidal size range, thus are also potential colloidal vectors of radionuclides. Microbial processes are discussed specifically in Section 5.7.
- Colloids that form at the front of migrating plume emanating from SFR, due to sharp gradients in the chemical conditions.
- Colloids that form at the redox front, due to sharp gradients in the chemical conditions. During temperate conditions, reducing conditions are expected at repository depth (see Sections 5.4 and 5.5) and so this redox front will lie above the repository.

Not all of these type of colloids are expected to come into contact with radionuclides, and are therefore of low relevance for radionuclide transport. Colloids formed downstream of SFR are of low relevance to the safety assessment.

Colloid stability. The concentration and persistence of any colloid depends on the extent to which it remains as a dispersed entity and avoids aggregation to the point of sedimentation or attachment to available surfaces. Repulsive forces are therefore required between colloids, and between colloids and surfaces. These forces are controlled by a number of factors including the pH, ionic strength and colloid density in solution. Colloids may also be removed from a system when chemical properties change (e.g. the transition from reducing to oxidising conditions may induce degradation reactions causing them to break down into their component molecules).

pH. The charge on most particle surfaces changes significantly with pH. At low pH, protonation tends to result in positively charged surfaces. As the pH increases, deprotonation lowers the charge until the surface reaches its point of zero charge (pzc), which can be determined experimentally. The pzc is depends not only on the chemical composition of the particle or mineral surface but also on factors such as the age and mode of formation. As the pH increases further from the pzc, the surface becomes negatively charged through further deprotonation and/or hydroxide ion association with surface sites. Most naturally occurring colloids possess a negative surface charge at pH 7, however some colloids such as hydrated iron and aluminium oxides can have a pzc as high as at pH 9 (van Loon and Duffy 2000). Clearly there will be greater repulsion between colloids with the same (positive or negative) surface charge, thus aggregation of a given colloid type will be greatest at the pzc. Likewise, the acidic functional groups in the structures of humic acids and analogous colloids are important in determining their stability with respect to aggregation. When these acid groups are deprotonated, the negative charges enhance the polarity of the humic acid, and thus its solubility in water. The enhanced intramolecular repulsions also lead to an expanded molecular volume. Conversely, more acidic conditions result in protonation of the acid groups, lowering the polarity of the macromolecule and causing contraction, aggregation and precipitation (Keepax et al. 2002).

Ionic strength. Dissolved ions can also interact with colloid surfaces and affect the surface charge and colloid stability. The main mechanisms are electrostatic adsorption (reversible ion-exchange process) and specific adsorption (covalent chemical bonding) onto surface binding sites (van Loon and Duffy 2000). Colloids are particularly unstable in the presence of divalent ions such as Ca^{2+} and Mg^{2+}, thus ion-exchange reactions involving Na^{+} and Ca^{2+} are important.

However, ionic strength also affects the stability of colloids through changes to the electric double layer surrounding the colloid. The electric double layer results from the electric field the colloid exerts on the surrounding solution. Close to the colloid, dissolved ions of opposite charge to the colloid surface (counter ions) experience electrostatic attraction, while those of the same charge experience repulsion. This generates a solution phase "layer" around the colloid with a predominance of counter ions. A common measure of the thickness of the electric double layer is the distance over which the electric potential has decreased to about 37% of its value at the colloid surface (van Loon and Duffy 2000). A higher ionic strength results in a higher density of counter ions around the colloid, thus the surface potential is lowered over a shorter distance and the thickness of the electric double layer is reduced. This, in turn, lowers the repulsive forces between colloids and leads to aggregation. The critical coagulation concentration (CCC) is the total cation concentration that results in diffusion-controlled aggregation of colloids, which results in rapid sedimentation.

For humic acids and other organic colloids, a high ionic strength also results in lower solubility, with neutralisation of the intramolecular repulsions as counter ions associate with the acid functional groups. As with a high H^+ concentration, this leads to contraction, aggregation and precipitation (Keepax et al. 2002). However, evidence suggests that humic substances do not aggregate under conditions that would destabilise inorganic colloids, and so are less sensitive to ionic strength conditions (Wold 2003)

Quantification of colloid stability. The Derjaguin–Landau–Verwey–Overbeek (DLVO) theory calculates colloid stability by summing the attractive van der Waals forces between colloids and the electrostatic repulsion generated by the electrical double layer at the colloid surfaces. When the attractive forces dominate over the repulsive forces, the colloidal particles tend to aggregate and become immobile due to sedimentation. When the repulsive forces dominate, the colloidal particles are stable and remain in solution. The temperature affects the electrostatic repulsion component of the equation in a complex manner (García-García et al. 2009).

Colloidal transport and filtering. Stable colloids in the geosphere may be transported with the flowing groundwater through fractures in the rock. The extent of transport depends on both the flow rate and the physical properties of the flow path and of the colloids. The physical properties determine the extent to which colloids are filtered out of solution. The main mechanisms of filtration are "pore straining attachment" when the colloids are too large to pass through the apertures, and "grain attachment" when colloids attach to solid surfaces through for example electrostatic, van der Waals, physical or hydrophobic interactions. These mechanisms are illustrated in Figures 5-1b and 5-1c, respectively. The width distribution of the pores, the presence and size distribution of other particles and the surface roughness of the pores affect the extent of colloid filtration. Narrow or blocked flow paths or paths densely populated by suspended particles limit colloid transport and rough, irregular pore surfaces enhance colloid removal from solution. Equally, larger, denser, irregular colloids will have more difficulty passing through narrow apertures. The dependency of overall transport on colloid size is complex due to dispersion effects (Wold 2010). Another process for colloid filtration is "ripening", which is the increase in pore surface roughness that results from colloid deposition and increases the likelihood of further colloid deposition. Ripening can lead to the blocking of pathways that are relatively wide with respect to the colloid size.

Colloids can attach reversibly onto mineral surfaces, for example by physical filtration or by electrostatic attraction, however, detachment may be hindered to varying extents by chemical or physical factors.

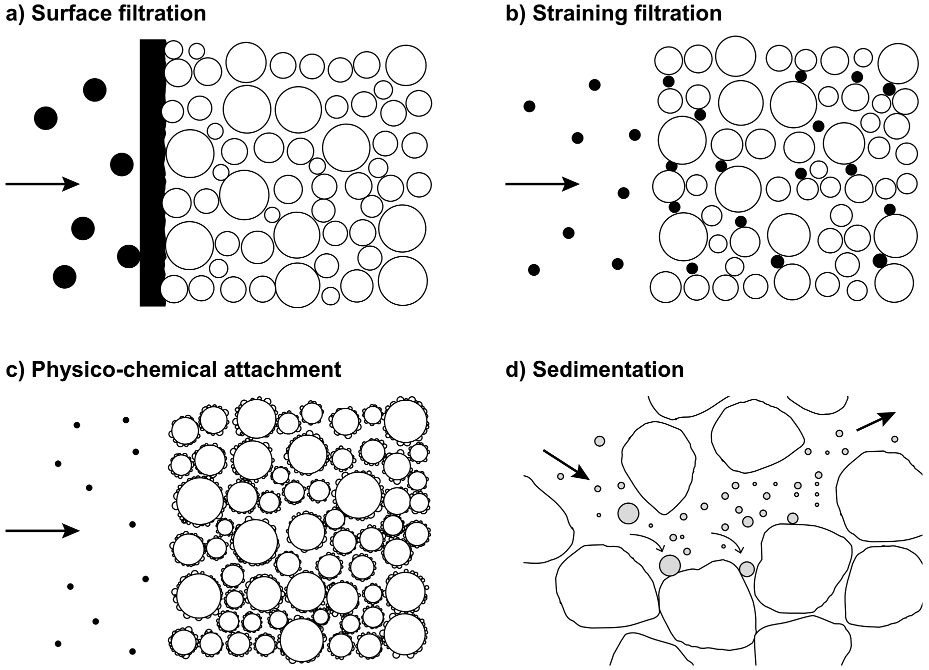

Figure 5-1. Illustration of different mechanisms of filtration (from Alexander et al. 2011).

Transport of reversibly attached colloids depends on the relative rates of attachment and detachment, which are affected by changes in chemical or hydraulic conditions. Sudden changes in chemical and hydraulic conditions have been found to mobilise a pulse of colloids in several studies (Laaksoharju et al. 1995, and references therein), however it was found that the large increase in dispersed colloid concentration was temporary.

In an unsaturated system, additional processes can contribute to colloid interactions with the pore surfaces. Limited water present in thin films over the solid phase can limit the ability of the colloid to move into the solution phase and gas bubble formation across a flow path can block colloid migration. However, colloids may also attach to gas bubbles through hydrophobic interactions and be transported by flotation. For gas transport, see Section 3.2. Due to the highly complex colloid–pore interactions, the simplified DLVO theory has been found to give a non-sufficient to satisfactory description of the retention or filtration of colloids along a flow path (Smith and Degueldre 1993).

5.9.2 Dependencies between process and geosphere variables

In this section, dependences between colloidal processes and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-15 outlines how colloidal processes are influenced by other geosphere variables, while Table 5-16 outlines how colloidal processes influence the defined geosphere variables. The influence between the process and each geosphere variable is elaborated upon below. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. Note that the handling for the periglacial and glacial climate domains as well as for the earthquake scenario has been omitted from the tables. Larger uncertainties in the repository function and contaminant transport in the geosphere exist during these periods, which negate the importance of colloid facilitated transport. The handling during these climate domains and events is therefore the same for all variables in that no radionuclide or colloid retention is accounted for in modelling. This handling is motivated by low consequence in the biosphere. The handling in the safety assessment SR-PSU for the excavation, operation, and saturation period as well as during the temperate climate domain is indicated in the rightmost column in the table. In Section 5.9.7, the handling for all time periods, climate domains, and events is elaborated upon in a discussion provided by the SR-PSU team.

In the analysis, the input of colloids from the waste and barrier system is considered a boundary condition for colloid facilitated radionuclide transport in the geosphere. These colloids have the greatest potential to transport radionuclides, but have been judged to be of low stability in the **Waste process report** and the **Barrier process report**. Natural colloids that remain outside the repository domain have less opportunity to interact with radionuclides, and can only facilitate the onwards migration of radionuclides that have already migrated out of SFR. Similarly, colloids that form at the redox/chemical front of the migrating leachate plume have limited opportunity to enhance radionuclide migration. Although most colloids are deemed to be of relatively low stability under leachate and current groundwater conditions, the low input of colloids from the SFR barriers and waste strengthens the rationale for neglecting the influence of colloid facilitated radionuclide transport in the geosphere.

Explanation of Table 5-15

Temperature in bedrock

Temperature affects colloid stability in a relatively complex manner according to DLVO theory.

Groundwater flow

The groundwater flow regime affects the rate of stable colloid transport and influences filtering through grain attachment. Higher flow rates may also enhance the formation of colloids through erosion.

Gas phase flow

Colloids can attach to the surface of gas bubbles and be transported with the bubbles.

Fracture and pore geometry

The size and surface character of the fractures and pores will affect the extent to which colloids interact with the fracture and matrix surfaces, i.e. are filtered.

Table 5-15. Direct influences of defined geosphere variables on the process "Colloidal processes" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.9.7)
Temperature in bedrock	Yes.	E/O/S, T	Temperature variations in the bedrock are negligible during temperate conditions. Furthermore, negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Groundwater flow	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Groundwater pressure	No		
Gas phase flow	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Repository geometry	No		
Fracture and pore geometry	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Rock stresses	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Matrix minerals	No direct influence. Colloids will not access the rock matrix due to pore size constraints and electrostatic repulsion.		
Fracture minerals	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Groundwater composition	Yes.	E/O/S, T	The groundwater composition is considered in the evaluation of colloid stability.
Gas composition	No.		
Structural and stray materials	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.
Saturation	Yes.	E/O/S, T	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate which therefore may be associated with radionuclides. Influence is neglected.

Rock stresses

Stress release in the rock, e.g. fracturing or rock fall-out, may generate colloids.

Fracture minerals

The fracture minerals will affect the extent to which colloids attach to the surfaces, i.e. are filtered. Fracture minerals may also contribute to colloid formation.

Groundwater composition

The groundwater composition (Eh, pH, ionic strength and dissolved organic materials) will affect colloid stability. Changes in the groundwater composition may generate colloids, e.g. at the migrating front of an alkaline plume from SFR.

Structural and stray materials

Structural and stray materials may contribute to the colloid population. Indirectly, they will also affect the colloid population by affecting the groundwater composition, although this effect would be negligible compared with the alkaline plume from the repository concrete.

Saturation

Gas phases may block colloidal flow paths and may prevent colloids dissociating from surfaces.

Table 5-16. Influences of the process "Colloidal processes" on defined geosphere variables, and a short indication of how this may be handled in safety assessment. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.9.7)
Temperature in bedrock	No.		
Groundwater flow	No.		
Groundwater pressure	No.		
Gas phase flow	No.		
Repository geometry	No.		
Fracture and pore geometry	Yes.	All	Negligible amounts of stable colloids are assumed, in particular those emanating from the repository leachate. Influence is neglected.
Rock stresses	No.		
Matrix minerals	No.		
Fracture minerals	Yes.	All	Negligible formation and amounts of stable colloids are assumed. Influence is neglected.
Groundwater composition	Yes.	All	Negligible formation and amounts of stable colloids are assumed. Influence is neglected.
Gas composition	No.		
Structural and stray materials	Yes.	All	Negligible formation and amounts of stable colloids are assumed. Influence is neglected.
Saturation	No.		

Explanation of Table 5-16

Fracture and pore geometry

The fracture and pore geometry could be affected by colloids if colloids attach to the fracture and pore surfaces in sufficient quantities.

Fracture minerals

The formation of colloids through erosion of fracture minerals could influence these volumes (amounts) minerals.

Groundwater composition

Colloid transport will influence the amount of colloids dispersed in the groundwater. Formation of colloids through precipitation, which occurs at a groundwater mixing front, may also change the dissolved composition of the groundwater.

Structural and stray materials

The formation of colloids from structural and stray materials may influence the amounts of these materials.

5.9.3 Boundary conditions

The boundary conditions for the concentration of colloids present (input and stability) are the exchange of colloids and dissolved species with the SFR wastes and barriers, and the biosphere. Boundary conditions for colloid transport are the groundwater flow rate and the dimensions of the fractures in the host rock.

5.9.4 Model studies/experimental studies

There have been a number of experimental studies investigating the stability and transport of colloids under variable conditions. While these support the general interactions described in the introduction, it should be noted that none of the studies are specific to the geosphere surrounding SFR or its colloidal population. Studies focused on cement colloids are discussed in the **Barrier process report**, and suggest that there will not be a significant input of these colloids into the geosphere.

The stability of colloids under the conditions expected in the groundwater of SFR and, more importantly, in the leachate plume emanating from SFR is an important consideration for the safety assessment. Wold (2003) examined the stability of Ca and Na forms of bentonite as a function of ionic strength, due to $CaCl_2$. Ca-bentonite and Na-bentonite colloids were suppressed at $CaCl_2$ ionic strengths of ~0.005 and ~0.01 M, respectively. The use of NaCl solution resulted in greater colloid stability, with suppression first observed at an ionic strength of 0.1 M. García-García et al. (2009) studied the stability of montmorillonite colloids under different ionic strength, pH and temperature conditions, and found that all three conditions affected the rate of colloid aggregation. Montmorillonite colloids were least stable at the lower pH values and higher temperatures and ionic strengths studied. However, the overall relationship with temperature was complex, because it influences both the intercolloidal repulsion and the collision frequency. The stability of colloids generated from vadose zone Hanford sediments have also been found to be suppressed by Ca^{2+} to a greater extent than by Na^{+} (Czigány et al. 2005). For humic acids, Wold (2003) characterised a critical coagulation concentration (CCC) of 0.1–0.5 M $NaClO_4$ in the initial pH range 3.9–9.7. The pH of the systems changed over the course of the experiments to between pH 5.9–7.9. Changes in the ionic strength below the CCC had no effect on the solution phase concentration or the mean size of the humic colloids. Wold (2003) also found that ionic strength had a marked influence on humic acid sorption to bentonite at pH 8; the K_d changed from 10 ± 10 cm^3/g in 0.01 M $NaClO_4$ to 180 ± 20 cm^3/g in 0.1 M $NaClO_4$. Despite this, experiments investigating diffusion of humic substances through bentonite in 0.01 M and 0.1 M $NaClO_4$ showed that the transport was largely unhindered (Wold and Eriksen 2007). Additionally, the presence of humic acid (0.1 g/L) altered the diffusion behaviour of Eu(III), so that it resembled that of the humic colloids.

The sorption of humic acid to goethite phases has also been shown to be higher at higher ionic strength and lower pH (Weng et al. 2007). This is consistent with the general understanding of humic acid solubility as a function of pH and ionic strength. However, the surface charge of the goethite is positive at low pH and negative at high pH, thus protons were found to be co-adsorbed with humic acid at pH 5.5 and above (in 0.1 M $NaNO_3$). Experiments investigating the transport of goethite colloids through quartz sand have also shown the importance of pH; at low pH colloidal goethite was strongly retained by the quartz, while at high pH greater colloid–quartz repulsion resulted in colloidal breakthrough that was consistent with predictions based on electrostatic interactions (Sätmark et al. 1996).

The transport of a colloid can also be affected by the sorption of humic acid to its surface, which alters its surface properties. Yoshida and Suzuki (2008) showed that humic acid enhanced the transport of aluminium oxide colloids at pH 6 and 8 through a quartz sand column. In the absence of humic acid, the positive zeta potential of the aluminium oxide and negative potential of the quartz resulted in favourable colloid–matrix interactions, hindering transport. The equilibration of negatively charged humic acid with the aluminium oxide prior to elution onto the column reduced the interactions with the matrix. At pH 8 and with 27 mg/L humic acid, aluminium oxide transported to the same extent as the humic colloids.

Colloid-mediated radionuclide transport has also been shown to depend on the strength of the radionuclide interaction with the colloids. Turner et al. (2006) demonstrated that illite colloids transport Cs more effectively than Sr through a quartz sand column, due to the slower desorption kinetics of Cs. Additionally, work has shown that humics can enhance Am(III) transport very significantly. At the lowest humic concentrations investigated (6 mg/L), 0.1% of Am(III) was transported as a mobile colloid after 7 days equilibration, and equilibration with higher humic concentrations enhanced this further (Artinger et al. 1998).

In addition the following discussion is extracted from the SR-Site process report (SKB 2010e) but is of relevance also to SFR:

In the colloid dipole experiment at the Grimsel test site, transport of radionuclides with and without bentonite colloids was studied in an injection–withdrawal experiment between two boreholes connected by a fracture. The experiment indicates that bentonite colloids enhance radionuclide transport (Möri et al. 2003b). However, the groundwaters at Grimsel are very dilute (~10^{-3} M ionic strength) and are therefore not representative for SFR conditions although alkaline conditions prevailed during the experiment (pH around 9). Under these experimental conditions, natural colloids and bentonite colloids are known to be very stable.

Colloid stability and transport of especially bentonite colloids in dilute water mimicking glacial water, on different scales, has been performed in the SKB Colloid Dipole Project, and is further carried on in the SKB Colloid Transport Project (García-García et al. 2006, 2007, Vilks et al. 2008). In the ongoing Grimsel Colloid Formation and Migration (CFM) project conducted at the Grimsel Test Site, bentonite erosion is studied on metre to field scales. The purpose is to investigate the influence of colloids on radionuclide migration in a fractured host rock under advective flow conditions at repository relevant conditions.

5.9.5 Natural analogues/observations in nature

Colloids in the current groundwater. Studies of colloids in granitic groundwaters in Sweden have focussed on the depths of relevance for the spent fuel repository. However, Hallbeck and Pedersen (2008a) measured a colloid concentration of 170 μg/L in a Forsmark borehole (KFM01A) at 112 m depth. The total range of measured colloid concentrations in Forsmark is 5–170 μg/L and the average is 58 μg/L (Hallbeck and Pedersen 2008a), and for Laxemar the range is 5–90 μg/L and the average is 24 μg/L (Hallbeck and Pedersen 2008b). In general, the groundwater at these sites has a relatively high ionic strength and high divalent cation concentrations, which are consistent with the low colloid concentrations observed. The colloid concentrations are comparable with those from studies of colloids in crystalline rock groundwaters in Switzerland (30 and 10 μg/L; Degueldre 1994).

More widely, saline and non-saline granitic groundwaters at 5 sites in Sweden (in the depth range 50–1600 metres) have been found to have median colloid concentrations of 20 and 45 μg/L, respectively (saline water min = 2 μg/L, max = 3000 μg/L), dominated by metal oxyhydroxides, silicate and clay mineral colloids (Laaksoharju et al. 1995). This analysis dismissed calcite and sulphide colloids as artefacts of the sampling procedure. The colloid concentration in the groundwater at Äspö hard rock laboratory decreased with salinity and depth, from a maximum of 3000 (70 m depth, low salinity) to < 50 μg/L (Laaksoharju 2003).

An earlier report examined humic acids in Swedish deep granitic groundwaters, and found that humic acids are typically present at 10^{-4} g/L (Pettersson et al. 1990). Humic and fulvic acid concentrations have not been determined in groundwater at depths representative of the SFR. Dissolved organic carbon (DOC) data, however, allow comparison of the groundwater organic composition at different depths, although only a small portion of the DOC consists of complex-forming humic and fulvic substances (Allard et al. 1991). DOC concentrations in the shallow groundwater (1.1–1.4 mg/L; at depths 4–119 m) of the SFR site (Lindquist and Nilsson 2010) fall into the range expected for typical Swedish deep granitic groundwaters (Allard et al. 1991).

Low colloid concentrations have also been observed at the Maqarin site, Jordan, at the natural cement/unaltered Marl host rock interface (Wetton et al. 1998).

5.9.6 Time perspective

In conjunction with closure of the repository, locally occurring colloid formation cannot be ruled out as a result of mixing of oxidising and reducing waters. Colloids formed are however judged to destabilise (coagulate) due to the high ionic strength of the leachates from different components at SFR and as reducing conditions are reinstated.

During the post-closure temperate period, reducing conditions are expected to prevail at repository depth. Colloid stability and formation in the repository and in the host rock at repository depth are then negligible mainly due to the high ionic strengths in the natural groundwaters and leachates from SFR components.

The stability of colloids would increase in dilute waters. During a glaciation, melt waters under the ice may intrude rapidly to repository depth due to elevated hydraulic gradients. If these waters contain large amounts of dissolved oxygen they will induce the oxidation of Fe(II) in near-surface waters, possibly resulting in colloidal Fe(III) oxyhydroxides (SKB 2010e). Although these melt waters are initially dilute, they are expected to acquire solutes by diffusion from the rock matrix and by reactions with fracture and matrix minerals present along the flowpaths, which could cause colloids to destabilise and sediment.

Nevertheless, the uncertainties in the repository function and integrity already during the periglacial permafrost, preceding the glacial melt water intrusion, negate the importance of colloid facilitated radionuclide transport.

5.9.7 Handling in the safety assessment

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

Colloids are not addressed in this period

Periods of the temperate climate domain

In this period, the high Ca concentration in the groundwater will suppress the stability of negatively charged inorganic colloids. Although changes in the groundwater chemistry arising from physical changes in the shoreline position may enhance inorganic colloid stability, evidence from less saline Swedish deep granitic groundwaters suggests they will not increase significantly. Additionally, the groundwater in the vicinity of SFR will be influenced by the concrete structures of the repository itself, resulting in high ionic strength, high Ca concentration waters. Therefore, the repository will destabilise inorganic colloids further in the geosphere (see the **Barrier process report**).

The plume arising from SFR will induce changes in the pH, ionic strength and eventually the redox conditions of the groundwaters in the geosphere, which will affect the stability of colloids, their interactions with surfaces and their formation (Laaksoharju et al. 1995). The migrating front of the water plume is expected to generate colloids, but this front will carry an insignificant proportion of SFR radioactivity. Therefore the effect of these colloids on radionuclide transport is also neglected in the safety assessment.

Although humic substances are likely to be much more stable than inorganic colloids under deep geological, repository influenced, conditions, they are not expected to be abundant at depth due to the low input of organic matter from the biosphere and are also neglected in the safety assessment.

Periods of the periglacial climate domain

During periglacial conditions water flow will be limited by the permafrost (frozen conditions), and therefore colloid facilitated transport is assumed negligible.

Periods of the glacial climate domain

Colloids will be most stable and be transported to the greatest extent in glacial melt water, due to its low ionic strength and low divalent ion concentration. However, the abundance and nature of colloids in this water is unknown, and will depend to a large extent on the water chemistry and the colloidal and chemical influence from SFR at that time, including the potential release of bentonite colloids from the Silo. For the glacial climate domain, the geosphere radionuclide transport model addresses enhanced transport of radionuclides regardless of the presence of stable colloids, and it is coupled to the scenario of loss of barrier function in the repository model (**Radionuclide transport report**). This handling for the glacial climate domain is motivated by low remaining radioactivity in the repository and therefore low consequence in the biosphere. Glacial melt water would also be expected to have low organic carbon content, and so the influence of humic substances is neglected.

Earthquakes

The impact of earthquakes on colloid-facilitated transport is not specifically addressed since geosphere retardation is conservatively disregarded in the analyses of impacts of earthquakes.

Handling relative to geosphere variables

Colloids are judged in SR-PSU to have a negligible influence on the transport of radionuclides in the geosphere, on the basis of the water chemistry and boundary conditions, and are not handleded explicitly.

5.9.8 Handling of 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.

The uncertainties discussed in the **Waste process report** regarding bitumen colloid stability are also relevant for colloidal processes in the geosphere.

Model simplification uncertainties

Colloidal processes in the geosphere are not modelled in SR-PSU.

5.9.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.10 Methane hydrate formation

In the SR-Site Geosphere process report, the process of methane hydrate formation is described (see SKB 2010e, Section 5.11 and references therein). It is recommended to study this text for a more elaborated description of methane hydrate formation, as well as for guidance to supporting references.

5.10.1 Overview/general description

Methane 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 methane trapped in cages of hydrogen-bonded water molecules (i.e. clathrates). Four conditions are required to form hydrates:

- low temperature (usually < 300 K),
- high pressure (> 38 bar hydrostatic pressure at 277 K),
- non-polar guest molecule smaller than 0.9 nm (i.e. methane), and,
- presence of water.

Figure 5-2 shows a phase diagram of the methane–water mixture as a function of pressure, shown as the equivalent depth, versus temperature (K). In the diagram a hydrostatic pressure gradient of 10^4 Pa/m is assumed as well as a site uncovered by an ice sheet. Methane hydrate is stable when the temperature is less than, or equal to, the line indicated by $T_3(P)$. This is further discussed in the SR-Site Geosphere process report (SKB 2010e, Section 5.11).

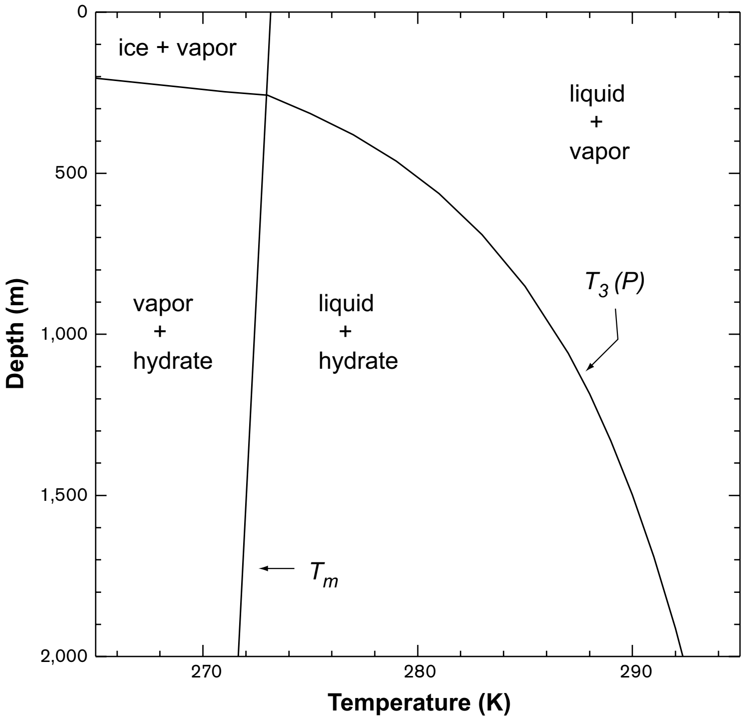

Figure 5-2. *Phase diagram for a methane–water mixture as a function of depth and temperature. Temperature $T_3(P)$ bounds the region where hydrate is stable and T_m is the melting temperature of pure water; after Buffett (2000). Reproduced from SKB (2010e, Figure 5-3).*

In the following, the four conditions in the above bullet list of formation requirements are discussed in the context of SFR; with emphasis on the fact that SFR is a shallow repository. Low temperatures are expected in the SFR repository and its surrounding host rock during periods of periglacial and glacial climate domains. However, the repository is situated in too shallow rock to facilitate the pressures required for methane hydrates to form, unless there is an extensive ice sheet above the repository. This means that for the repository, at the depth of the rock vaults, the process is only of interest during glacial periods. For the SFR site, during the SR-PSU assessment time scale, it can be questioned whether an ice sheet will form (see the **Climate report**).

In the rock mass deeper than ~200 m, methane hydrates can also form during periods of periglacial climate conditions without the presence of an ice sheet, as a result of the increased hydrostatic pressure at depth (cf. Figure 5-2). For SFR, at least for the initial phase, the presence of methane in the repository and its surroundings predominantly originates from the decomposition of the waste (see the **Waste process report**). In the host rock, minor amounts of methane may also originate from natural sources. In comparison with the KBS-3 repository, it is safe to say that there may be a larger amount of methane gas associated with SFR. Concerning the presence of water, this is a prerequisite normally fulfilled in SFR and its host rock.

The formation of methane hydrates in porous spaces, such as fractures, upon lowering the temperature or increasing the pressure, may block flow paths. This may lead to an altered flow pattern. The formation of the hydrates may also lead to mechanical alteration of the pore space and surrounding material (e.g. fracturing). This would have a similar effect as the formation of regular ice (H_2O) during permafrost conditions. Although the 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 gas at 1 atm and 273 K. Upon decreasing the pressure or increasing the temperature to certain values (see phase diagram in Figure 5-2), the hydrates become unstable. Where dissociation of the solid methane ice occurs, giving rise to methane gas, there will be a volume change that may affect conditions in the rock and in the repository, especially if large quantities are transformed at the same time.

In the perspective of SFR, the temperature in the repository will during permafrost conditions decrease to such levels that water will freeze (see Section 2.2 and the **Climate report**). The freezing of water may also occur in the porous system of structural material such as concrete, if the temperature is well below zero. The effect will be structural degradation, which below a certain temperature may be extensive. Glacial periods, where the increased pressure from the ice sheet would allow for the formation of methane hydrates, are preceded by permafrost conditions, see the **Climate report**. Therefore, structural degradation similar to that associated with methane hydrate formation will likely already have occurred, by the formation of regular ice. Similar reasoning applies for the fracture system of the host rock surrounding SFR. Possibly, at larger depths to which permafrost does not reach, additional fracturing due to hydrate formations is conceivable. However, at such depths the host rock experiences little effect from the methane production in the repository and should resemble the rock discussed in the SR-Site Geosphere process report. There it was concluded that hydrate formation is not possible at the reported natural methane concentrations and water salinities (SKB 2010e, Section 5.11.7).

In the SFR repository, methane hydrates may form and subsequently become unstable, leading to dissociation of methane gas. As discussed above, the formation requires high pressures, which in the case of SFR could be achieved by the hydrostatic pressure from an ice sheet, in addition to the regular hydrostatic pressure at repository depth. When the ice sheet melts, and the pressure decreases below a certain value (cf. Figure 5-2), the hydrates become unstable and it is conceivable that large amounts of gas will form, which may in turn affect the water flow out of the repository and into the geosphere. At this point in time, that is when the ice sheet is melting; the repository would likely be covered by a warm based ice sheet. In such a case, the presence of the melting ice sheet would anyhow increase the water flow rate through the repository and geosphere. Consequently, the melting of the ice sheet and the resulting melt water flow would likely overshadow the effect on the groundwater flow imposed by dissociation of methane hydrates. Furthermore, if the methane gas production would lead to an increased rate of radionuclide transport out of the repository, such a release would be much diluted by the glacial melt water. It is conceivable that gaseous radionuclides, predominantly ^{14}C-methane, can be carried with the presumed methane gas pulse out of the geosphere system. If so, the gas pulse is likely to dissipate into the atmosphere without the methane being incorporated in the biomass at the surface (as this is during the glacial period). Furthermore, a glacial period would be so far in the future that most of the C-14 would have decayed.

5.10.2 Dependencies between process and geosphere variables

In this section, dependences between the methane hydrate formation process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. Table 5-17 outlines how the process is influenced by the defined geosphere variables, while Table 5-18 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event the described influence occurs. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is a brief description of the handling of the influence in the safety assessment SR-PSU. In Section 5.10.7, this handling is discussed.

In Table 5-17, only the glacial time periods are handled, implicitly meaning that methane hydrates will not form in the SFR repository host rock (if limiting the host rock down to a depth of 200 m) during the temperate or periglacial climate domains. Nor has the process any consequence for earthquakes. If not limiting the host rock to a depth of 200 m, the process can also occur during the periglacial climate domain (see Table 5-18).

Table 5-17. Direct influences of defined geosphere variables on the process "methane hydrate formation" and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviation: G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.3.7)
Temperature in bedrock	Yes.	G	Generic assessment of the possibility of methane hydrate formation is performed, based on e.g. Figure 5-2.
Groundwater flow	No, but indirectly through: Groundwater composition.	G	–
Groundwater pressure	Yes.	G	Generic assessment of the possibility of methane hydrate formation is performed, based on e.g. Figure 5-2.
Gas phase flow	Yes. By bringing or removing the gas to/from the regime of methane hydrate formation/dissociation.	G	No limitations in hydrate formation due to limitations in gas phase flow assumed in the generic assessment.
Repository geometry	No.	G	–
Fracture and pore geometry	Yes. Hydrates form in fractures and voids of the rock mass.	G	No limitations in hydrate formation due to limitations in fracture geometry assumed in the generic assessment.
Rock stresses	No, but indirectly through: Fracture and pore geometry.	G	–
Matrix minerals	No, but indirectly through: Temperature (through thermal properties of rock matrix).	G	–
Fracture minerals	No.	G	–
Groundwater composition	Yes. Dissolved salts lower the equilibrium temperature $T_3(P)$ in Figure 5-2. Methane concentration is crucial.	G	The inhibiting effect on hydrate formation (in the presence of gas) due to an increased salinity is pessimistically neglected in the generic assessment. The methane concentration is assumed not to be limiting.
Gas composition	Yes. The concentration of methane is crucial.	G	Unlimited access to methane is assumed in the generic assessment of the possibility of methane hydrate formation.
Structural and stray materials	No.	G	–
Saturation	Yes Water is needed for the process.	G	Saturated and liquid phase conditions in the bedrock are assumed.

Explanation of Table 5-17

Temperature in bedrock

According to Figure 5-2 the temperature is a crucial condition for the formation and dissociation of methane hydrates.

Groundwater flow

Groundwater flow may transport dissolved methane and heat, thus affecting the possibility of methane hydrate formation.

Groundwater pressure

According to Figure 5-2 the pressure is a crucial condition for the formation and dissociation of methane hydrates.

Gas phase flow

Gas phase flow may bring the methane gas to, or remove the gas from, the regime of methane hydrate formation or dissociation.

Repository geometry

The repository geometry, with the exception of repository depth, does not directly affect the potential for forming methane hydrates in the geosphere.

Fracture and pore geometry

Methane hydrates form in fractures and voids in the rock mass. Their presence is therefore a prerequisite for their formation. Also, the adsorptive capacity of the rock affects the process by lowering the freezing temperature. Therefore, the fracture aperture, which affects the average distance to the fracture surfaces, may be of relevance.

Rock stresses

Changes in in situ rock stresses, here due to the varying ice sheet thickness, may change the fracture and pore geometry. This is not thought to have a significant effect at the conditions where methane hydrates form or dissociate.

Matrix minerals

Indirectly, matrix minerals affect the rock temperature by way of their thermal properties.

Fracture minerals

It is conceivable that the electric charge of fracture mineral surfaces could affect the conditions for formation and dissociation of methane hydrates; just as it affects the freezing temperature of regular ice. However, such intricate dependencies are outside the scope of SR-PSU.

Groundwater composition

The groundwater composition affects the conditions (in terms of salinity) where the formation of methane hydrates can occur. A saline groundwater would provide less favourable conditions for hydrate formation, as compared to a non-saline groundwater. Needless to say, the methane concentration affects the potential for methane hydrate formation.

Gas composition

The methane concentration (impacting the methane distribution between gas phase or as dissolved) affects the potential for methane hydrate formation.

Structural and stray materials

The structural and stray materials do not directly affect the potential for forming methane hydrates in the geosphere.

Saturation

Water is needed for methane hydrate formation. However, water is always abundant at depth, except under frozen conditions.

Table 5-18. Direct Influences of the process "methane hydrate formation" on the defined geosphere variables, and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviations: P = Periglacial climate domain. G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.3.7)
Temperature in bedrock	Yes. By latent heat of formation/dissociation.	P/G	The influence of methane hydrate formation/dissociation on the temperature is neglected.
Groundwater flow	Yes. By changing flow path geometries and gradients.	P/G	Possible changes in water flow path geometries (due to formation) and gradients (due to dissociation) are neglected.
Groundwater pressure	Yes. Upon rapid dissociation.	P/G	Possible short-lived changes in pressure gradients (due to dissociation) are neglected.
Gas phase flow	Yes. When methane dissociation occurs.	P/G	An increase in gas phase flow (due to dissociation) is neglected in SR-PSU.
Repository geometry	No.	P/G	–
Fracture and pore geometry	Yes. Methane hydrates may open up or expand fractures.	P/G	Potential alteration of fracture geometry due to methane hydrates below 200 m depth, or during glaciation, is neglected.
Rock stresses	Yes. By expansion of the methane hydrate ice.	P/G	Such changes in rock stresses are neglected.
Matrix minerals	No.	P/G	–
Fracture minerals	No.	P/G	–
Groundwater composition	Yes. The formation of methane hydrates would deplete surrounding groundwater from methane. Also, salt exclusion may occur.	P/G	This effect of methane hydrate formation on groundwater composition is neglected.
Gas composition	Yes. Formation and dissociation of methane hydrates affects the fraction of methane in the gas phase.	P/G	An increased or decreased methane fraction in the gas phase, as result of this process, is of no consequence for SR-PSU.
Structural and stray materials	Yes. The formation of methane hydrate may degrade cementitious materials.	G	Such materials are expected to already have degraded prior to the glacial period.
Saturation	Yes. Dissociation of methane hydrates can cause localised and short-lived unsaturation of the fracture system.	P/G	This is neglected.

Explanation of Table 5-18

Temperature in bedrock

The latent heat of formation/dissociation of methane hydrates may locally affect the bedrock temperature, but only to a negligible degree.

Groundwater flow

If methane hydrate ice blocks fractures, this would likely alter the flow paths in a manner similar to the formation of regular ice under permafrost conditions. Methane ice formation could occur below the depth of 200 m but also at shallower depth during glacial periods. At depths below 200 m, the effect from methane formation in the repository host rock should be small and the groundwater composition should resemble that of the host rock for the KBS-3 repository. In SR-Site, it was judged that the formation of methane hydrates is unlikely as a result of the low concentrations of methane, in combination with the salinity levels at depth. In case of methane hydrate dissociation, expanding gas may create a very temporary driving force for groundwater.

Groundwater pressure

Hydrate formation may in some instances affect the groundwater pressure, if the system is closed or poorly connected, or temporarily upon rapid methane dissociation. In order for a non-temporary change to occur, water would have to be 1) hindered to move away from the forming gas at a sufficient rate, implying a poorly connected fracture system; or 2) trapped in a fracture by the expanding ice giving rise to a very local effect.

Gas phase flow

In case of stable methane hydrate ice; this may block gas phase flow paths below the depth of 200 m, or at the depths of SFR during glacial periods. Upon dissociation of methane hydrates, should they form in the first place, the gas phase flow would be increased by the release of methane.

Repository geometry

Methane hydrate formation is not related to changes in repository geometry. At the time methane hydrates may form in the direct vicinity of the repository, rock fallout is assumed to already have occurred (to the limited degree of fallout generally expected).

Fracture and pore geometry

The expansion of methane hydrate ice may open up or expand fractures, or otherwise "damage" the rock surrounding SFR. This effect is likely overshadowed by the effect of regular ice (H_2O) formation at repository depth.

Rock stresses

Expanding methane hydrate ice (relative to the water volume from which it was formed) may cause rock stresses to increase, to a negligible degree.

Matrix minerals

The formation of methane hydrates is not expected to directly influence matrix minerals.

Fracture minerals

The formation of methane hydrates is not expected to directly influence fracture minerals.

Groundwater composition

The formation of methane hydrates would deplete the surrounding groundwater from methane. Also, salt exclusion may occur in a similar process as described in Section 5.11 for the formation of H_2O ice.

Gas composition

Methane dissociating from the hydrates would affect gas composition by way of increasing its methane concentration. On the other hand, the formation of hydrates depletes groundwater from methane.

Structural and stray materials

The expanding methane hydrate ice may degrade porous cementitious structural and stray material in the same manner as the formation of regular ice. However, the degradation due to regular ice will already have occurred prior to the first glacial period, as an effect of permafrost.

Saturation

The dissociation of large amounts of methane from the hydrates would result in large quantities of gas, resulting in localised and short-lived unsaturation of the fracture system of the rock.

5.10.3 Boundary conditions

The exchanges of methane and of heat with the repository, surface systems, and with deep parts of the geosphere comprise boundary conditions for the formation and subsequent dissociation of methane hydrates. Methane hydrates can only form in certain temperature and pressure regimes (see Figure 5-2). Climate changes will lead to changes in surface temperatures and heat-transfer parameters, and also to increased/decreased water pressures in case of the formation and subsequent melting of an ice sheet. Consequently, the hydrostatic pressure is an additional boundary condition.

5.10.4 Model studies/experimental studies

This and the next section are largely reproduced from the SR-Site Geosphere process report. Because of the economic importance of gas hydrates as a future energy source, there is an abundance of experimental and model data published in the open literature, for example, comparing laboratory-derived synthetic clathrate hydrates with those naturally formed (Stern et al. 2004). Understanding the alteration of naturally occurring hydrates may help to unravel their in situ state or growth processes. For example, Circone et al. (2004) addressed the effect of elevated methane pressure on methane hydrate dissociation. Several textbooks describe the formation and stability of methane hydrates, for example (Sloan and Koh 2007).

Modelling simulations were carried out to assess the risk of methane hydrate formation during future permafrost conditions at candidate sites for a final repository for spent nuclear fuel in Sweden and Finland (Bahman et al. 2010). The main conclusion is that there is no risk of hydrate formation at the reported methane concentrations and water salinities.

5.10.5 Natural analogues/observations in nature

Several sites presently under permafrost conditions have been, or are, in the process of being investigated. These include crystalline rocks in Canada (e.g. Ruskeeniemi et al. 2002, 2004, Stotler et al. 2009, Holden et al. 2009), deep sedimentary rocks in Russia (e.g. Alexeev and Alexeeva 2003), and sea sediments in Canada (e.g. Dallimore and Collett 1995, 1999, Clark et al. 1999). Of the many observations documented, the Mallik sea sediments in the MacKenzie Delta, Northwest Territories, Canada, represent the first concerted effort to study the occurrence of natural gas hydrates in a permafrost environment. The objectives were to obtain geological, geophysical, and geochemical data of the Mallik gas hydrate field and to perform production testing of a concentrated gas hydrate reservoir. The physical behaviour of the hydrate deposits was monitored after depressurisation and thermal stimulation. Gas-hydrate-bearing core samples were collected and down-hole geophysical logging was performed. In parallel, detailed laboratory experiments were conducted providing greater physico-chemical understanding of the formation, stability, and ultimate dissociation of these hydrate phases under similar permafrost conditions to those expected during future climate change in Fennoscandia.

No methane hydrates have been found during the Lupin Mine studies, but indicators of their past presence were noted by Stotler et al. (2009). This included the identification of possible areas beneath the permafrost layer where mine-induced depressurisation is thought to have resulted in melting of methane hydrates, contributing to the dilution observed in some subpermafrost groundwaters.

5.10.6 Time perspective

Methane hydrates may only form in the vicinity of the SFR rock vaults during glaciation, should such occur within the assessment time frame. Below about 200 metres depth, they may also form during the periglacial periods, given the right conditions.

5.10.7 Handling in safety assessment

In this section, the handling of methane hydrate formation is described. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-17 and Table 5-18 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

Methane hydrate formation cannot take place during this period.

Periods of the temperate climate domain

Methane hydrate formation cannot take place during these periods.

Periods of the periglacial climate domain

Methane hydrate formation cannot take place at repository depth during these periods. While temperature and pressure conditions may favour methane hydrate formation below the depth of about 200 m, it is judged that such formation is unlikely (Bahman et al. 2010). At depth, the methane concentration should not be significantly influenced by the methane production in the SFR repository, and the situation should resemble that of the KBS-3 repository host rock. In SR-Site, it was judged that the formation of methane hydrates was not possible as a result of low concentrations of methane, in combination with the salinity levels at depth (SKB 2010e). The same judgement is made for the SFR host rock below 200 m. In summary the consequence is judged to be negligible and no further handling is recommended for SR-PSU.

Periods of the glacial climate domain

The nature of some of the waste in SFR would allow for the formation of methane, even if such production is assumed to predominantly occur prior to the onset of the next glacial period (see the **Waste process report**). If assuming elevated methane concentrations, in combination with low temperatures and an increased pressure as result of ice sheet overriding, this would allow for the formation of methane hydrates in the host rock fractures, and more so within the repository vaults. However, as such hydrates cannot form in the rock fractures under permafrost conditions (as the fractures are already filled with ice); this would require a warm based ice sheet and degraded subglacial permafrost conditions. The formation of methane hydrates may degrade cementitious structural materials in the same manner as regular ice formation. However, such materials are assumed to already have degraded prior to the onset of the next glacial period, during previous permafrost episodes. Accordingly, the consequence of methane ice formation is judged to be negligible and no further handling is performed in SR-PSU.

As discussed in Section 5.10.1, already formed hydrates at repository depth may dissociate as the ice sheet melts and the pressure decreases below a certain level. The possible dissociation of large amounts of methane from the hydrates would result in large quantities of gas, which would have consequences for the gas flow and conceivably also for the groundwater flow. Concerning the latter issue; during the melting of the ice sheet, when the front of the ice sheet is fairly close to the repository, groundwater flows are already elevated. This would mask the potential effect of methane dissociation on the groundwater flow. Therefore the consequence is judged to be negligible and no further handling is performed in SR-PSU.

Earthquakes

While earthquakes may possibly trigger a destabilisation of accumulated methane hydrates, as discussed in the SR-Site Geosphere process report (SKB 2010e, Section 5.11.7), the formation and destabilisation of methane hydrate should be of little consequence for the onset of an earthquake at the Forsmark site.

Handling relative to geosphere variables

Temperature in bedrock

The influence of methane hydrate formation on the rock temperature is neglected in SR-PSU, as the hydrates will not form at repository depth during permafrost conditions, and as the bedrock temperature is of greatest consequence for permafrost modelling in relation to the repository depth. Moreover, the latent heat of formation/dissociation of methane hydrates is judged to be too small to have a significant effect on the general bedrock temperature.

Groundwater flow

The potential influence of methane hydrate dissociation in the underground openings, or in the vicinity of underground openings, during the melting of the ice sheet has been neglected in hydrogeological modelling and argumentation. This is justified as the potential influence on the water flow would be masked by the increased water flow resulting from the melting ice sheet.

Groundwater pressure

The formation and dissociation of methane hydrates should not affect the groundwater pressure in the relatively well connected SFR host rock, except perhaps momentarily and localised. This is judged to be of no consequence for the safety of SFR.

Gas phase flow

The dissociation of methane hydrates may have a short-term effect on the gas phase flow. The magnitude of the gas flow during glacial periods is not of direct concern for the safety of SFR. No detailed gas phase flow modelling is performed for the geosphere in SR-PSU.

Repository geometry

No direct dependency between the repository geometry and methane hydrate formation has been found, with the exception for the repository depth. As the process is generally deemed as insignificant for repository safety, it does not contribute to the choice in repository depth.

Fracture geometry

The expansion of methane hydrate ice may affect the fracture system and "damage" the surrounding rock. However, in the shallow host rock of SFR, such damage is already expected to have occurred as result of the formation of normal ice (H_2O) during permafrost conditions. Accordingly, such a potential effect is neglected in SR-PSU.

Rock stresses

The expansion of methane hydrate ice may affect the stress situation of the surrounding rock, to a very limited degree. However, this would be of little consequence for the SFR repository given the fact that methane hydrates require an ice sheet to form. During such conditions, the rock stress changes of consequence are induced by the overburden of the ice sheet.

Matrix minerals

The formation and dissociation of methane hydrate would not affect matrix minerals.

Fracture minerals

The formation and dissociation of methane hydrate would not affect fracture minerals.

Groundwater composition

The process will not affect the groundwater composition at repository depth during temperate and periglacial climate domains. During the melting of the ice sheet, the inflow of meltwater into the geosphere would mask any potential effects of methane hydrate formation and dissociation (with the possible exception of the methane concentration in the groundwater). The consequence is judged to be negligible for repository safety and no further handling is performed in SR-PSU.

Gas composition

Upon dissociation of methane hydrates, the presence of methane would of course affect the composition of a gas phase. However, this is judged to be of no consequence for repository safety. The risk of explosions that would affect repository safety is judged to be negligible.

It is conceivable that small amounts of ^{14}C-methane gas can be carried with the presumed methane gas pulse out of the geosphere system. If so, the gas pulse is likely to dissipate into the atmosphere without the ^{14}C-methane being incorporated in the biomass at the surface (as this is during the glacial period). Accordingly, this is neglected in SR-PSU.

Saturation

In SR-PSU, fully saturated conditions are assumed in the host rock at depth. This may briefly and locally be changed by the presence of flowing methane gas. However, as this should have no long-term effect, the assumption of fully saturated conditions is judged to be appropriate.

5.10.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Methane ice formation is a physically well understood process.

Model simplification uncertainties

No numerical modelling of methane hydrate formation or dissociation is performed in SR-PSU. The generic assessment of the possibility of methane hydrate formation, made in this present section, is based on reasoning and data shown in Figure 5-2.

In the assessment made in this section, one can say that it is a simplification to assume that the methane production in the repository does not affect the methane contents of groundwaters below 200 m depth. However, in case methane exists in free gas phase, this gas should not flow downwards.

It may also be seen as a simplification to assume that the effect of methane hydrate dissociation on the groundwater flow is masked by the increased flow resulting from the melting of the ice sheet. In support of this it is argued in Section 3.3 that in general, gas phase flow has limited effect on the groundwater flow.

5.10.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.11 Salt exclusion

Salt exclusion may affect the groundwater in the host rock surrounding the SFR repository by similar processes as for the KBS-3 repository. Therefore, the text composed for the SR-Site Geosphere process report (SKB 2010e, Section 5.12) is to a large extent relevant. However, the implications of salt exclusion for the two repositories differ. For one thing, permafrost has been estimated not to reach the KBS-3 repository depth (SKB 2010b), whereas SFR is situated at such a shallow depth that the permafrost may reach down to, and below, the present repository and the planned extension.

This shifts the focus of salt exclusion for SR-PSU, compared to SR-Site. On the one hand, more attention is paid to discussing what happens with the melt water of the permafrost, or perennially frozen ground, which has been depleted of solutes by salt exclusion. On the other hand, less attention is paid to the potential for brine formation at greater depth. For this latter issue the reader is encouraged to consult (SKB 2010e, Section 5.12).

5.11.1 Overview/general description

When water freezes slowly, the solutes present in the water will not be incorporated in the crystal lattice of the ice. As a consequence, the water surrounding the forming ice will increase in solute concentration. The efficiency of the freeze-out process is dependent on e.g. the available amounts of solutes in the unfrozen water and the efficiency of the freezing process. When permafrost (i.e. the 0°C isotherm) and perennially frozen ground form, they develop from the ground surface and downwards (see Section 2.2). In this process, a propagating freezing zone constitutes a gradual transition from unfrozen conditions to conditions with progressively smaller unfrozen water content, resulting in a vertical distribution of unfrozen water within the permafrost (see Figure 5-3).

The occurrence of this freezing zone is due to the fact that freezing of water takes place over a range of temperatures, depending on groundwater salinity, ambient hydrostatic pressure, and the aperture of the water-containing pores and fractures.

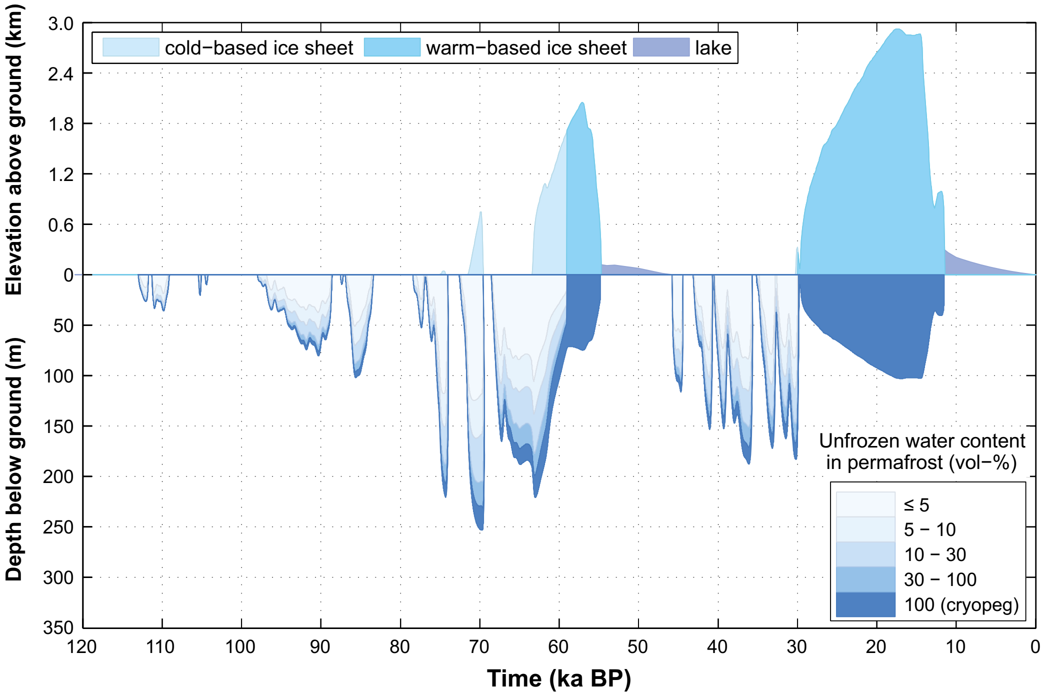

Figure 5-3. Unfrozen water content in the permafrost for the reference glacial cycle (SKB 2010c). The heat from the KBS-3 repository has been included in the permafrost simulations, whereas no heat is produced from SFR. The reduction in permafrost and freezing depths over SFR, introduced by the presence of the nearby KBS-3 repository, are however not large, on the order of a few tens of metres at maximum.

During freezing, salts that have been present in the surface waters and groundwaters may accumulate in and below the propagating freezing zone. The freezing process could, under certain circumstances and if repeated a number of times to a similar depth, give rise to a boundary between fresh and saline water at the depth to which freezing has reached. However, such a boundary is not expected to appear at the Forsmark site (see the **Climate report**).

Modelling results from SR-Site indicate that when the salt transport occurs more slowly than the freezing zone advances, salinity concentrations are increased within the perennially frozen ground (Hartikainen et al. 2010). Depending on the general gradual character of the propagating freezing zone, and on the geometry of the groundwater-containing fracture system, pockets of unfrozen saline waters could, at least temporarily, become confined within the perennially frozen bedrock.

At the shallow depth of SFR, permafrost is assumed to develop repeatedly in several of the climate cases (see Section 2.2 and the **Climate report)**. Depending on the extent of the permafrost, this may cause the freeze-out zone to be above, at, or below repository depth at different time periods.

Studies made for SR-Site showed that freezing can induce salt exclusion and transport at the Forsmark site when perennially frozen ground develops deeper than ~200 m (Hartikainen et al. 2010, Section 5.1 and Conclusions). However, the results further showed that at more shallow depths, the impacts of freezing in terms of salt-exclusion are difficult to see because of the low salinity content of the shallow groundwater prior to the development of perennially frozen ground.

The results further show that the climate required to make the freeze-out process efficient needs to be considerably colder than the one reconstructed for the last glacial cycle (Hartikainen et al. 2010, Section 5.1). Furthermore, generic simulations carried out by Vidstrand et al. (2006) suggest that a regional groundwater flow beneath a permafrost layer would cause a “flushing” of the rejected salt and hence dilute the salinity. Based on the above discussions and results, the effect of salt exclusion is considered negligible for the shallow SFR repository at Forsmark.

In the crystalline rock at the Forsmark site, only a few percent of the rock’s total water content exists in the fracture system. The rest of the water exists in the microporous network of the rock matrix (e.g. Crawford 2008, SKB 2010b). This can be exemplified by assuming a typical fracture aperture of 0.1 mm, and a porosity of the fracture adjacent rock of 0.5%. The water volume in the fracture equals only that contained in the first centimetre of bounding rock. The free water in the fractures freezes at a higher temperature than the constrained water in the microporous system of crystalline rock, due to differences in pore aperture, even if the two waters have similar compositions (Wessman 1997). If fracture water becomes more concentrated below or within the freeze-out zone, as discussed above, it will initially be surrounded by less concentrated matrix pore water whereto (part of) the surplus of solutes can diffuse. This would lessen the effect of salt exclusion on the fracture water composition. Even as the freeze-out zone has passed and the fracture water is frozen, solutes can diffuse further into the microporous system of the rock matrix. If the groundwater has begun to freeze, forming a freezing zone, this would prevent a vertical flow of water and, consequently, the replenishing of solutes from surface waters. The microporous system could accordingly buffer the effect of salt exclusion as a result of freezing groundwater. As only a fraction of the total groundwater exists in fractures, and the great majority exist in the rock matrix, one would expect only a moderate increase in the pore water concentration, as a result of the added solutes.

In a separate case, large quantities of brackish or marine surface water could freeze. If the body of surface water is constrained, this may result in significant volumes of residual and highly saline surface water. This water may penetrate down into the host rock in unfrozen fracture zones, as its density is higher than the existing groundwater. In this case, the quantity of the water that is affected by salt exclusion is not restricted by the volume of the fracture system. Hence, the volume (and transport properties) of the micropores of the rock matrix may not be sufficient to offer a buffering effect. However, this case is not expected at the SFR site, at least not at the relatively shallow repository depth, as the site is expected to be situated inland at periods of the periglacial climate domain (see the **Climate report**). Consequently, the site is not expected to be covered by brackish or marine surface water.

When the permafrost retreats and the ice in the fractures melt, the melt water is initially much diluted. This may be of consequence for the repository in terms of barrier degradation (see the **Barrier process report**). However, as the volume of the dilute melt water is small compared to the volume of the surrounding pore water, diffusion from the rock matrix to the fractures should quickly replenish the supply of solutes in the fracture water. Furthermore, fracture and rock minerals may undergo water interactions resulting in dissolution (and alteration), which would also add solutes to the melt water. Consequently, the fracture adjacent rock will present a buffering effect towards diluted melt waters, as the permafrost retreats.

Freeze-out processes have been used to explain some of the saline lake occurrences in the extreme climatologically conditions of Antarctica, where it was referred to as 'freeze-drying' or 'freeze concentration' (Matsubaya et al. 1979, Burton 1981). Since then, the contribution of a freeze-out process has been discussed in relation to the deep Canadian Shield brines (e.g. Herut et al. 1990, Bottomley et al. 1994, 1999, Starinsky and Katz 2002), where the chemistry of the brines may reflect both evaporative and cryogenic processes. In the context of Fennoscandia, Bein and Arad (1992) proposed that bedrock saline groundwaters present in coastal areas of the Baltic Sea are the result of the freezing of seawater which may have occurred just prior to the over-riding of a marine body by an ice sheet. In general, if 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 under certain circumstances produce residual waters of greater salinity, or in extreme cases even of brine character (> 100 g/L TDS). However, when modelling the Forsmark site with its specific setting, the results indicate the absence of such highly saline residual water (Hartikainen et al. 2010). Neither has water of highly saline/brine character been found in the Forsmark and SFR site investigations (Laaksoharju et al. 2008b, SKB 2013b), to the depth investigated.

5.11.2 Dependencies between process and geosphere variables

In this section, dependences between the process of salt exclusion and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-19 outlines how the process is influenced by the defined geosphere variables, while Table 5-20 outlines how the process influences the defined geosphere variables. Furthermore, it is indicated during what time period, climate domain, or event the described influence is valid. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is a brief description of the handling of the influence in the safety assessment SR-PSU. In Section 5.11.7, this handling is elaborated upon in a discussion provided by the SR-PSU team.

In Table 5-19 and Table 5-20, only the periglacial and glacial time periods are handled, implicitly meaning that salt exclusion will not take place during the temperate climate domain. Neither has the process any consequences for earthquakes, or vice versa.

Explanation of Table 5-19

Temperature in bedrock

The temperature in the bedrock affects the groundwater temperature and thus the possibility for freezing. This in turn affects the freeze-out process and the extent of salt exclusion.

Groundwater flow

The groundwater flow affects the groundwater composition, for example by way of removing the accumulating salts in case of salt exclusion. The groundwater flow also affects the groundwater temperature and hence the possibilities of freezing and salt exclusion.

Groundwater pressure

The groundwater pressure affects the freezing temperature of water, and thus the freeze-out zone and salt exclusion.

Table 5-19. Direct influences of defined geosphere variables on the process "salt exclusion" and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviations: P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.11.7)
Temperature in bedrock	Yes. Temperature affects freezing.	P/G	Bedrock temperature is handled in permafrost modelling (see Section 2.2).
Groundwater flow	No, but indirectly through: Temperature and groundwater composition.	P/G	2D groundwater flow is included in permafrost simulations.
Groundwater pressure	Yes. Pressure affects freezing temperature of water.	P/G	Groundwater pressure is included in permafrost modelling (see Section 2.2).
Gas phase flow	No.	P/G	–
Repository geometry	No.	P/G	–
Fracture and pore geometry	Yes. Fracture geometry affects pathways for freeze-out zone. Matrix diffusion lessens the effect of salt exclusion.	P/G	Results from SR-Site modelling are used, so details in the fracture and pore geometry are not accounted for.
Rock stresses	No.	P/G	–
Matrix minerals	No, but indirectly through: Temperature and groundwater composition.	P/G	–
Fracture minerals	No, but indirectly through: Groundwater composition.	P/G	–
Groundwater composition	Yes. Affects the salts that may be frozen out, and freezing temperature of water.	P/G	Groundwater salinity is included in permafrost modelling (see Section 2.2).
Gas composition	No.	P/G	–
Structural and stray materials	No.	P/G	–
Saturation	Yes.	P/G	Fully saturated conditions are assumed.

Gas phase flow

The thermal energy of flowing gas has a negligible influence on the freezing of groundwater.

Repository geometry

The salt exclusion is not directly affected by the repository geometry.

Fracture and pore geometry

The large-scale fracture geometry influences the overall pathway for the freeze-out zone and the accumulating salts. The fracture volume may, under certain circumstances, also restrict the amount of groundwater that can freeze, and thus the amount of accumulating salts. Related to the small-scale geometry; the adsorption of water molecules on fracture mineral surfaces lowers the freezing temperature. At larger fracture apertures the importance of this effect decreases, as the average distance to either of the fracture surfaces is increased. In the micropores of the rock matrix, where the pore apertures are very small, the pore water freezes at lower temperatures than the groundwater in the fractures (if it freezes at all).

In the case of salt exclusion in fractures, the solutes may diffuse into the microporous system of the rock matrix and thereby reduce the concentrating effect of the salt exclusion. The reverse effect applies upon melting of the permafrost ice (see Section 5.11.1).

Rock stresses

The salt exclusion is not directly affected by the rock stresses, even though the rock stress may affect the fracture and pore geometry.

Matrix minerals

Heat transport will predominantly take place by conduction in the rock mass. The thermal conductivity of the matrix minerals therefore affects the temperature of the rock and groundwater, and thus also indirectly the freeze-out zone. Matrix minerals are also important for the groundwater composition, which affects the freezing process.

Fracture minerals

Fracture mineral dissolution and precipitation associated with the freeze-out will influence the groundwater composition and therefore indirectly the salt exclusion. Furthermore, the adsorption of water molecules on mineral surfaces decreases the freezing temperature, and thus indirectly salt exclusion. However, this effect should be fairly similar for different types of common minerals. If part of the fracture is directly bounded by matrix minerals, the adsorption of water molecules on such mineral surfaces has a similar effect.

Groundwater composition

The groundwater composition determines the amount of salt that can be excluded from the forming ice. Also, the composition affects the water's freezing temperature, as more saline water freezes at lower temperatures (see Section 2.2).

Gas composition

Salt exclusion is not directly affected by the gas composition. To some extent the gas (e.g. CH_4) may dissolve and change the groundwater composition, and thereby indirectly affect the freezing (see Section 5.10).

Structural and stray materials

Structural and stray materials should not significantly affect the freeze-out zone in the geosphere. However, this is under the prerequisite that the structural and stray materials do not extensively alter the (local) groundwater composition. In such a case, there is an indirect influence via groundwater composition. Here it should be recalled that the amount of structural and stray materials is very small compare to the amount of foreign materials in the repository vaults.

Saturation

The degree of saturation affects the freezing and thus the salt exclusion. However, fully saturated conditions are assumed in the repository host rock. The exception is for very shallow rock, such as outcrops, and Quaternary deposits that fall outside the framework of this **Geosphere process report**.

Explanation of Table 5-20

Temperature in bedrock

The process of salt exclusion in itself (that is the redistribution of solutes) will not affect the bedrock temperature.

Table 5-20. Direct influences of the process "salt exclusion" on the defined geosphere variables, and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviations: P = Periglacial climate domain, G = Glacial climate domain.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.11.7.
Temperature in bedrock	No.	P/G	–
Groundwater flow	Yes. Salinity affects density driven flow.	P/G	Density driven flow, as result of salt exclusion, is not accounted for in SR-PSU hydrogeological modelling.
Groundwater pressure	Yes. Salinity affects density and thus groundwater pressure.	P/G	The effect is neglected in SR-PSU, as the effect on salinity is judged to be very small.
Gas phase flow	No.	P/G	–
Repository geometry	No.	P/G	–
Fracture and pore geometry	No.	P/G	–
Rock stresses	No.	P/G	–
Matrix minerals	No, but indirectly through: Groundwater composition.	P/G	–
Fracture minerals	No, but indirectly through: Groundwater composition.	P/G	–
Groundwater composition	Yes. By way of altering the salinity (groundwater composition) in association with the freeze-out zone.	P/G	The impact of salt exclusion on groundwater composition at repository depth is judged to be very limited, partly based on SR-Site modelling.
Gas composition	No.	P/G	–
Structural and stray materials	No.	P/G	–
Saturation	No.	P/G	–

Groundwater flow

Saline waters have higher density and will, to some extent, influence groundwater flow by gravitational effects.

Groundwater pressure

Saline waters have higher density and will, to some extent, influence groundwater pressure by gravitational effects.

Gas phase flow

Salt exclusion will not affect the gas phase flow.

Repository geometry

Salt exclusion will not affect the repository geometry.

Fracture and pore geometry

Salt exclusion will not affect the large-scale fracture geometry. However, precipitates of fracture minerals, or dissolution of fracture minerals, may to a minor extent affect the local fracture geometry.

Rock stresses

Salt exclusion will not affect rock stresses.

Matrix minerals

Salt exclusion will not affect fracture distant matrix minerals to a significant extent, as the process should only induce reasonably small changes in the pore water composition at SFR (which may in turn somewhat affect the stability of the minerals and their surface properties). Adjacent to the flowpath, similar precipitation/dissolution reactions as for fracture minerals may occur, as result of the change in groundwater composition.

Fracture minerals

Salt exclusion may indirectly affect fracture minerals through groundwater composition, since production of saline waters may lead to precipitation of new phases at the fracture surfaces. Also, fracture minerals may dissolve in the diluted permafrost melt water. Such precipitation/dissolution is expected to be minor.

Groundwater composition

Salt exclusion directly affects the groundwater composition, by increasing solute concentrations in the groundwater in and below the freeze-out zone, and by facilitating diluted permafrost melt water.

Gas composition

Salt exclusion will not affect the gas composition.

Structural and stray materials

Structural and stray materials may degrade at slightly different rates in waters of different salinities. However, as the changes in salinity are expected to be very limited, salt exclusion will not influence the structural and stray material degradation rates at a significant degree. Also, at the time salt exclusion may occur, structural and stray materials are expected to already have degraded.

Saturation

Salt exclusion will not affect the degree of saturation.

5.11.3 Boundary conditions

The compositions and quantities of the surface- and groundwater, and the temperatures at the ground surface and in the rock, comprise the boundary conditions for the freezing of shallow waters, with resulting salt exclusion. The large scale groundwater flow is also a boundary condition, as it may carry away solutes at or below the freezing zone. Saline surface water may also flow down into the host rock.

Climate change may lead to changes in surface temperatures and water compositions, which in turn may lead to the formation of permafrost and perennially frozen ground over long periods of time with the consequent exclusion of salts.

Small scale boundary conditions include the groundwater composition and pore aperture, which affects the freezing temperature. The pore water of the rock matrix presents a sink/source for solutes associated with salt exclusion.

5.11.4 Model studies/experimental studies

The freeze-out hypothesis is largely based on laboratory experiments related to sea water freezing where, for example, Nelson and Thompson (1954) were able to distinguish between the products of evaporation and freezing. The solid products from evaporation consisted of halite with subsidiary gypsum, and from freezing, hydrahalite and mirabilite. The most important difference during freezing is the removal of the SO_4^{2-} ion in mirabilite ($Na_2SO_4 \cdot 10H_2O$). However Marion et al. (1999), based on theoretical model and experimental evidence, demonstrated that gypsum also can precipitate spontaneously after mirabilite and at lower temperatures during sea water freezing, arguing that its inclusion is the most thermodynamically favoured pathway and close to that earlier proposed by Gitterman (1937). Moreover, from a theoretical point of view, depending on the Na/Ca ratio of the groundwater type present prior to permafrost activity, gypsum may be the first precipitated phase during freezing instead of mirabilite.

The 'freeze-out' concept, as described and discussed by Bein and Arad (1992), assumes that the formation of permafrost in a brackish lake or a restricted coastal sea environment (e.g. similar to that of the Baltic Sea or Hudson Bay in Canada) produced a layer of highly concentrated salinity ahead of the advancing freezing zone. Since this saline water would be of high density, it subsequently would sink to lower depths (i.e. density driven intrusion), would avoid dilution by oceanic water, and potentially penetrate into the bedrock where it would eventually mix with formational groundwaters until the density of the mixtures became similar to that of the existing groundwater at the current elevation.

Where the bedrock is not covered by brackish lake or constrained sea water, similar freeze-out processes may occur in the bedrock on a much smaller scale within the hydraulically active fractures and fracture zones, again resulting in formation of a higher density saline component in the residual fluids. The incremental downward propagation of the freeze-out zone will eventually cease due to increased salinity, increased temperature, and a decrease in transmissivity that will hinder potential pathways for the residual fluids.

Recent work (Ruskeeniemi et al. 2004, Zhang and Frape 2003, Zhang et al. 2006) describes freezing experiments using waters other than seawater; a Na–SO_4 groundwater from Palmottu, Finland and a Ca–Cl groundwater from Sudbury, Canada. In common with the seawater experiments, with progressive freezing all ions in the residual solutions showed an increasing trend towards greater concentrations. In addition, $\delta^{18}O$ and δ^2H became increasingly depleted. Compared with the Baltic and Canadian Shield brines, the resulting residual solutions from the freeze-out experiments generally plot at a higher sulphate concentration for a specific chloride concentration. Two mechanisms occurring in situ were invoked to explain this disparity: a) sulphate was removed as mirabilite, and b) sulphate was removed by microbial reduction to sulphide. Both processes are considered possible under permafrost conditions.

5.11.5 Natural analogues/observations in nature

Many studies have been reported from sites throughout the Canadian Shield (mostly deep mine localities) and these are adequately referenced in Bottomley et al. (1999) and Gascoyne (2000). Evidence for permafrost in crystalline rock environments was specifically addressed in the Palmottu natural analogue study (Blomqvist et al. 2000) and since then has been a focus of attention in studies of the Lupin Mine, Canada (Ruskeeniemi et al. 2002, 2004, Stotler et al. 2009), High Lake, Canada (Holden et al. 2009) and in the various site characterisation investigations being carried out in Sweden and Finland (e.g. Laaksoharju et al. 2008b, 2009). A large number of methane hydrate studies have also referred to the presence of residual fluids from ion exclusion during ice formation at the base of the permafrost layer (Torres et al. 20011). Studies of permafrost in crystalline bedrock are also performed within the Greenland Analogue Project (GAP) executed in western Greenland (SKB 2010g, Harper et al. 2011). The permafrost depth within this study area, adjacent to the ice sheet, is around 300 m. A 700 m deep borehole has been drilled through the permafrost and instrumented for hydrological sampling and detailed thermal measurements. The Lupin Mine studies have now been concluded, and while freezing processes are inferred to have occurred (e.g. the possibility of methane hydrate formation), the degree to which the freezing has modified the chemistry of the site has been difficult to quantify (Stotler et al. 2009). This difficulty has been compounded by the nature of the site, where there is widespread contamination due to long-term mining activities and also mixing of different groundwater types beneath the permafrost layer.

Mixing of different groundwater types has also plagued interpretation of the hydrochemical data from the Swedish sites, but some indication of freezing processes may have been preserved, especially at the Laxemar site (Laaksoharju et al. 2008b, 2009). The isotopes of oxygen, boron, and chlorine can be sensitive to freeze-out conditions, either becoming enriched in the ice phase (^{18}O and ^{37}Cl) or in the residual fluid phase (^{11}B). These isotopes have been investigated in the Laxemar groundwaters, in particular the brackish-glacial type, which mostly occurs at intermediate depths (about 300–600 m) and appears to have been reasonably well preserved in bedrock that shows a decrease in hydraulic conductivity with increasing depth. The data show enrichment in ^{11}B which has accumulated in most of these groundwaters and may be a result of freeze-out processes. In addition, the distribution of δ^{37}Cl shows a weak correlation between increasing enrichment of ^{37}Cl corresponding to a depletion of δ^{11}B in the same groundwaters, supporting also a possible freezing effect. Furthermore, two samples in particular show enriched ^{11}B together with depleted ^{18}O and possibly depleted ^{37}Cl, which may suggest a modification of the isotope systems related to freeze-out processes.

A number of porewater samples from depth intervals of about 430–550 m and 620–750 m at Laxemar show accumulated Na–Ca–SO_4 compositions. The origin of this sulphate is not clear, but possible sources are dissolution of gypsum and/or modifications induced by freezing processes.

In conclusion, whilst there is some support for freeze-out processes having occurred at Laxemar (less so at Forsmark), the degree to which the freezing has modified the chemistry of groundwaters, in common with the Lupin Mine studies, has not been possible to quantify.

5.11.6 Time perspective

Salt exclusion due to freezing may only occur under periods of perennially frozen ground conditions.

5.11.7 Handling in safety assessment

In this section, the SR-PSU team gives a description of how the process of salt exclusion is handled. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-19 and Table 5-20 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

Salt exclusion by freezing will not take place during this period.

Periods of temperate climate domain

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

Periods of periglacial climate domain

The permafrost modellings performed in SR-Site (SKB 2010c) and SR-PSU (Brandefelt et al. 2013), as reported in the **Climate report**, show that permafrost repeatedly will affect the host rock at the Forsmark site within several of the climate cases considered in the SR-PSU safety assessment. Since SFR is situated at a shallow depth, permafrost and perennially frozen ground can reach to repository depth and below. Site-specific calculations produced for SR-Site, showing the evolution of salinity within and below the freezing zone, have been used to evaluate the possible impact at and above repository level (~500 m) for the KBS-3 repository (Hartikainen et al. 2010). The results indicate that 1) salt exclusion at depths above 200 m is very limited due to low initial salinity, and 2) if salt transport occurs more slowly than the freezing zone advances, solute concentrations are increased within the perennially frozen ground (Hartikainen et al. 2010). Similar, but generic, simulations have been made by Vidstrand et al. (2010a, b). The 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 zone is not formed (Vidstrand et al. 2006), in line with the second conclusion above from Hartikainen et al. (2010).

From the above it can be concluded that a groundwater of greater salinity, as a result of salt exclusion, is unlikely at the SFR repository depth. Furthermore, hydrogeological modelling shows that the topography governs the groundwater flow pattern in the shallow rock, rather than density driven flow (cf. Section 3.2). Therefore, more concentrated groundwater at shallow freeze-out zones would soon become diluted as the permafrost thaws. Also, as discussed in Section 5.11.1, solutes of more concentrated water would diffuse into the rock matrix pore water, which would lessen the effect of salt exclusion.

As the freeze-out zone is likely to pass the repository, it is conceivable that when the ice melts, dilute melt water may contact the repository barrier (and waste) components. If so, this could possibly be of consequence for the degradation of, for example, the bentonite buffer around the silo. However, as discussed in Section 5.11.1, the amount of frozen water in the fracture system is limited in comparison to the amount of pore water of the rock matrix. Solutes would thus be supplied to the melt water by matrix diffusion (in addition to the dissolution/alteration of fracture minerals). Also, this melt water would be mixed with other waters as the permafrost retreats. Furthermore, cementitious materials from the engineered barriers are likely to supply solutes to the dilute water. For this reason, it is judged as unlikely that the limited amount of permafrost melt water should be of consequence for the safety of the repository. Based on the descriptions and reasoning in this section, it is judged that salt exclusion needs no further handling in SR-PSU, and that it can be disregarded.

Periods of glacial climate domain

The same reasoning as for periods of the periglacial climate domain applies for periods of the glacial climate domain. Also, for this climate domain it is judged that salt exclusion needs no further handling in SR-PSU, and can be disregarded.

Earthquakes

No relation between earthquakes and salt exclusion by freezing has been identified.

Handling relative to geosphere variables

Temperature in bedrock

The temperature in the bedrock is an important output from the modelling of permafrost, as presented in the **Climate report**. Through the permafrost modelling, temperature data are integrated in the assessment of consequences of salt exclusion.

Groundwater flow

In the SR-PSU hydrogeological modelling, with regard to density driven flow, a potential increase or decrease in salinity associated with a freeze-out zone is neglected. This is in line with the recommendations of this section, as such an increase or decrease would be minor.

Groundwater pressure

The groundwater pressure in the bedrock is an input to the modelling of permafrost depths (see Section 2.2). Through the permafrost modelling, groundwater pressure data are integrated in the assessment of consequences of salt exclusion.

Gas phase flow

No direct dependency between gas phase flow and salt exclusion has been found.

Repository geometry

No direct dependency between repository geometry and salt exclusion has been found.

Fracture and pore geometry

No detailed modelling of the freeze-out zone or salt exclusion that would require fracture and pore geometry data, is carried out in SR-PSU, as justified above. The exchange of solutes from the groundwater to the pore water of the rock matrix is used to argue that the consequence of salt exclusion is limited. A prerequisite for this is large-scale micropore connectivity, which is argued for in SKB (2010b, Section 6.8). Another prerequisite is a sufficiently large pore water volume, compared to the fracture water volume, which is the case in the bedrock at the Forsmark site (unless there is intrusion of large volumes of saline surface water).

Rock stresses

No direct dependency between rock stress and salt exclusion has been found.

Matrix minerals

No direct dependency between matrix minerals and salt exclusion has been found.

Fracture minerals

No change in fracture mineral abundances or compositions, due to precipitation associated with salt exclusion, is modelled in SR-PSU.

Groundwater composition

Changes in groundwater composition as a result of a freeze-out are judged to be of limited consequence, as justified above in this section. As a result, salt exclusion needs no further handling in SR-PSU hydrogeochemical modelling, and can be disregarded.

Gas composition

No direct dependency between gas composition and salt exclusion exists, with the possible exception of methane hydrate formation (see Section 5.10).

Saturation

The host rock is assumed to be fully saturated at the relevant times periods in SR-PSU.

5.11.8 Handling of uncertainties

Uncertainties in mechanistic understanding

The process of salt exclusion due to freezing is well understood. Also the interactions of solutes in the fracture water and rock matrix pore water are well understood. However, there is uncertainty concerning the extent to which permafrost has influenced the salinity of groundwaters found at repository depths at Swedish sites.

A mechanistic uncertainty lies in to what extent (part of) the pore water in the microporous system will freeze. Based only on the pore apertures and mineral properties, such a freezing should be possible at sufficiently low temperatures (Wessman 1997). However, due to the volumetric expansion associated with the freezing, the pore water pressure should increase, at some point preventing freezing of the remaining trapped pore water. This is in line with the conclusions from calculations of hypothetical freezing temperatures, and associated pressure increases, in confined buffer erosion cavities for a KBS-3 repository (SKB 2010c, Appendix 3).

Model simplification uncertainties

No modelling of salt exclusion is performed in SR-PSU, but results are adapted from SR-Site modelling (SKB 2010b). The argument made that salt exclusion should be of little consequence for repository safety is based partly on these results, but also on qualitative reasoning. As the overall judgement is made that the process of salt exclusion can be neglected in the safety assessment, the uncertainty from model simplifications should be small.

5.11.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

5.12 Earth currents

5.12.1 Overview/general description

Earth currents, that is electric currents, are common in natural systems such as soil and rock. Such currents may have both a natural cause and may result from anthropogenic activity. A number of natural and anthropogenic sources are listed in the SR-Site Geosphere process report (SKB 2010e, Section 5.13) and references therein. Furthermore, for a comprehensive background on anthropogenic and natural earth currents, Lanzerotti and Gregori (1986) is recommended. While earth currents from natural sources are direct, or have very low frequencies, anthropogenic earth currents may be both direct and alternating.

Earth currents may affect the transport of solutes, particles, colloids, and macromolecules in water saturated natural systems. They may also enhance the corrosion of metallic components in the repository and its surroundings, such as rock reinforcements. Both from the perspective of transport and corrosion (that also involves transport); direct currents are of much greater consequence than alternating currents. The reason is that direct currents can aid the transport of solutes, particles, etc over long distances, which may also facilitate reaction. Alternating currents, on the other hand, may only cause the solutes, particles, etc to “vibrate” on the same location. Consequently, this present section has direct currents as a focus of attention.

For the Forsmark site, the presence of the nuclear power plant and the closely located Fenno-Skan High Voltage Direct Current (HVDC) transmission creates a situation of relatively large earth currents, with a significant direct component. This creates measurable electrical potential gradients in the host rock, even at depth. In Nissen et al. (2005), local electrical potential gradients in the range of about 10 to 100 mV/m were measured at a depth of about 200 m at the Forsmark site (see Section 5.12.4). In the same report, it is stated that in the surroundings of Forsmark, the (large-scale) potential gradient is believed to be 300 mV/km.

It is wide-spread knowledge that earth currents may cause extensive corrosion (e.g. Lanzerotti and Gregori 1986, SKB 2010d, e). For the SR-PSU safety assessment, enhanced corrosion rates of engineered metallic components in the geosphere (i.e. rock reinforcements) are of little consequence, as those components are assumed to corrode quickly even in the absence of earth currents (SKB 2008c). Accordingly an enhanced corrosion of the rock reinforcements, which may potentially results in quicker rock fallout, would have little consequence for the safety assessment.

For the evaluation of the geosphere in the SR-PSU safety assessment, the direct consequence of earth currents, if any, would be associated with enhanced transport of charged solutes, complexes, and colloids in the groundwater and pore water. Such transport would occur through three different processes.

- Electromigration, where ionic solutes migrate in the electric field.
- Electrophoresis, where electrically charged particles, colloids, and macromolecules migrate in the electric field.
- Electro-osmosis, where ionic solutes, charged particles, etc drag water molecules with them in the electric field. This induces a water flow that may also cause transport of non-charged solutes.

All of these processes may influence the transport of radionuclides, either as dissolved or as associated with complexes or colloids. Except for the direct influence on radionuclide transport, earth currents facilitate transport of non-active solutes, complexes, and colloids. In the context of the main constituents of the groundwater, the overall transport is too minute to be of consequence for the repository safety. However, the process may affect the distribution of tracer elements between the fracture water and pore water of the rock matrix.

Electromigration is the most important transport mechanism for propagating earth currents through saturated crystalline rock, unless the electric field is alternating at a high frequency. Out of the processes in the above bullet list, it is probably also the most important transport mechanism for radionuclide transport and retention in crystalline rock. By electromigration, ionic solutes are transported through the water with an electrical potential gradient as the driving force. The transport occurs both in the groundwater of discrete fractures and in the pore water of the microporosity of the rock matrix[10]. In many instances, the electromigratory contribution from mobile cations counteracting the negatively charged mineral surfaces of the rock matrix is significant (e.g. Löfgren et al. 2009). The available water volume in the microporosity of the rock matrix is generally greater than that in water-bearing fractures. Accordingly, a substantial part of the electric current is transported through the non-fractured rock matrix. There is sometimes a misconception that a great majority of the earth current is propagated in water-conducting fractures, as rocks are poor electrical conductors (e.g. Miller et al. 2002, p 41). However, even though unsaturated crystalline rock is a poor conductor, saturated non-fractured rock conducts electric current reasonably well, with an electrical resistivity on the order of 10^4 ohm.m. If comparing the capacity of the non-fractured rock matrix with that of water-conducting fractures, they majority of the electric current is likely transported in the rock matrix, possibly with a significant contribution from water-bearing fractures that do not transport water. It should be noted than only an insignificant fraction of the current is conducted through mineral grains by electronic conduction, as they generally have a very high electrical resistivity (e.g. Schön 1996).

As the greater part of the electric current is transported through the rock matrix, it means that the electric field is not generally focused to discrete and water-conducting fractures. Therefore, there is no apparent relation between the direction of the water flow and that of the electric current. As a result, in case of radionuclides being transported by an advective flow in the fracture system, as solutes or complexes of limited size, electromigration will force them to leave the water stream and migrate into the stagnant water surrounding the flow path. This process strongly resembles radionuclide retention due to matrix diffusion (see Section 5.3). In fact, diffusion and electromigration are analogue processes where the solute's ionic mobility and diffusivity are related by the Einstein relation (e.g. Atkins 1998). The effect of the electrical potential gradient on radionuclide transport and retention would thus be an enhanced transport into the microporous system, which would result in greater retention.

In Löfgren and Neretnieks (2006), ionic tracers were transported through a 12 cm long granitic rock sample in the laboratory, using an electrical potential drop of about 40 V as the driving force. In this experiment the electro-migratory flux through the sample was about 1,500 times larger than the steady state diffusive flux through the same sample would have been, if using the same tracer solution. In the experiment, a potential gradient of about 330 V/m was used, which should be compared to the 10 to 100 mV/m local potential gradients measured in situ at the Forsmark site. The electro-migratory flux should reasonably well scale linearly with the electrical potential gradient. Accordingly, one can draw the conclusion that with the measured present day electrical potential gradients at the Forsmark site, the electro-migratory flux into the rock matrix would roughly be on the same order of magnitude as the diffusive flux. If removing the anthropogenic contribution to the earth currents, for example by closing the nuclear power plant and removing the HVDC transmission, the electromigratory flux would be negligible.

Electrophoresis involves charged particles and colloids, as well as macromolecules such as proteins and complexes of very large size. For example, a particle of clay exhibits a negatively charged surface and will move in an electric field relative to a stationary solution. As the particle is surrounded by counter ions in the diffuse double layer, these will slow the particle movement (e.g. Stumm and

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[10] By the terminology used there, the rock matrix includes matrix minerals as well as the microporosity constituted by grain boundary pores, micro-fractures, etc.

Morgan 1996). As electrophoresis affects relatively large particles, colloids, etc., the process cannot take place in the microporous network of the rock matrix, due to size exclusion. Therefore, the process can only act on radionuclides in the fracture water. In flowing fracture water, advection is the dominant transport mechanism. Accordingly, in such water electrophoresis can be neglected. One could argue that electrophoresis could have a retardation effect if moving radionuclides from the flow paths to stagnant parts of the fracture water. However, it is hard to quantify such an effect.

Electro-osmosis refers to the movement of the solvent relative to a stationary charged surface (Stumm and Morgan 1996). When solutes, particles, etc move, they drag the polar water molecules with them. In the case of negatively charged mineral surfaces in crystalline rock, there is a surplus of cations in the diffuse double layer that balance the negative mineral charge. When these cations move, the will drag part of the pore water with them. Löfgren and Neretnieks (2006) measured the electro-osmotic flow in crystalline rock (using a high potential gradient) and found it to be only a fraction of the electro-migratory flux through the same rock sample. As the electro-migratory flux into the rock matrix is expected to be roughly on the same order of magnitude as the diffusive flux, or less, one can disregard electro-osmosis in the rock matrix as an important transport mechanism. Electro-osmosis can also occur in the fracture water. However, compared to advection in flow paths and diffusion in stagnant parts, this can be neglected.

5.12.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 5-21 outlines how the process is influenced by the defined geosphere variables, while Table 5-22 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event the described influence is valid. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is a brief description of the handling of the influence in the safety assessment SR-PSU. In Section 5.12.7, this handling is elaborated upon in a discussion provided by the SR-PSU team.

Explanation of Table 5-21

Temperature in bedrock

The ionic mobility of solutes in the groundwater is slightly affected by the temperature (e.g. Atkins 1998). The part of the earth current which is conducted through mineral grains can be neglected. Therefore, the influence of temperature of mineral conductivity can be neglected. If the water freezes, it cannot propagate earth currents at any significant rate, and not by way of transporting charged solutes, particles, etc.

Groundwater flow

Generally, the flow of electric currents through the rock mass is independent of the direction and magnitude of the groundwater flow. An unbalanced advective flow of cations and anions (made possible by the negatively charged fracture mineral surfaces and surplus of dissolved cations) could give rise to minute electrical potential gradients. However, these can be neglected in the discrete fractures due to the relatively large fracture apertures (lowering the influence of the cation surplus in the electrical double layer).

Groundwater pressure

In an incompressible medium such as water, the groundwater pressure has no practical implications for the ionic mobility.

Gas phase flow

Earth currents are not propagated in gas. Therefore, the flow of electric current through the rock mass is independent of the gas phase flow, as long as the fractures still contain some water.

Table 5-21. Direct influences of defined geosphere variables on the process "earth currents" and a brief description of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation and saturation, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ=Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.12.7)
Temperature in bedrock	Yes. Temperature affects the ionic mobility and, thus, earth currents.	E/O/S T/EQ	Changes in ionic mobility due to changes in temperature are small and are neglected.
		P/G	Earth currents cannot be propagated in frozen water at significant rates.
Groundwater flow	No. Not significantly.	All	–
Groundwater pressure	No.	All	–
Gas phase flow	No.	All	–
Repository geometry	Yes. The repository affects the electric field in host rock.	All	Effect of repository is neglected, concerning earth current in the host rock.
Fracture and pore geometry	Yes. The processes take place in fractures and pores.	All	Electromigration occurs in fractures and micropores, as accounted for in assessment of retention contribution.
Rock stresses	No, but indirectly through: Fracture and pore geometry.	All	–
Matrix minerals	Yes. Minerals and mineral surface interactions affect earth currents.	All	Natural earth currents (from e.g. reaction) are neglected. Surface conductivity effects are indirectly accounted for in assessment of retention contribution.
Fracture minerals	No. Not significantly	All	–
Groundwater composition	Yes. Electrical conductivity of water affects earth currents.	All	The rock resistivity (partly as result of groundwater/pore water composition) is accounted for in assessment of retention contribution.
Gas composition	No	All	–
Structural and stray materials	Yes. Galvanic coupling could create local earth currents.	All	The effect of galvanic coupling is neglected.
Saturation	Yes. Earth currents are almost exclusively propagated in water.	E/O/S	Unsaturated conditions affect earth currents. This is not accounted for.
		T/P/G	Fully saturated host rock is assumed.

Repository geometry

The excavated repository, which contains more porous materials than the host rock, will have a lower resistivity (if saturated) than the surrounding rock. This affects the local electric field. This may give rise to local effects in the direct vicinity of the repository.

Fracture and pore geometry

The greater part of the electric current is propagated in the pore water of the microporous network in the rock matrix. A fraction is also propagated in fracture water, depending on how fractured the rock mass is (e.g. Löfgren and Neretnieks 2005). Electrophoresis only occurs in fracture water, due to size exclusion effects in the micropore network.

Rock stresses

Rock stresses may slightly compress fractures and micropores (Skagius and Neretnieks 1986). This would somewhat increase the rock resistivity and decrease the earth currents.

Matrix minerals

At the Forsmark site, an insignificant part of the current is conducted through mineral grains by electronic conduction, as the site is poor in ores. However, a substantial part is propagated by surface conduction in the pore water, as affected by the charged mineral surfaces (e.g. Crawford 2008).

Electrochemical reactions with minerals can also create local earth currents. However, this process is normally associated with ore bodies (e.g. Parasnis 1997), which should be rare in the Forsmark area.

Fracture minerals

Fracture minerals comprise a too low volume fraction of the rock mass to have a significant impact of the rock resistivity. The exception would be a wide spread abundance of highly conductive fracture minerals, such as pyrite. This is not the case at the Forsmark site (Eklund and Mattsson 2009, Löfgren and Sidborn 2010).

Groundwater composition

As earth currents are predominantly propagated by ionic solutes in water phase, the concentration of these solutes matters for the rock resistivity. The groundwater content of colloids and macromolecules affects the electrophoresis. However, electrophoresis should contribute little to the total amount of electric current propagated through the rock mass.

Gas composition

Earth currents are not propagated in gas.

Structural and stray materials

Structural and stray materials may affect the local pore water chemistry of the rock matrix, but not to such an extent that it has a significant impact on the general rock resistivity. Electrochemical reactions with (metallic) structural material can also create very local currents through galvanic coupling, but these are not considered as important for the general electric field in the host rock.

Saturation

As earth currents are almost exclusively propagated in water, the degree of saturation matters. At depth, fully saturated conditions can be assumed shortly upon repository closure.

Explanation of Table 5-22

Temperature in bedrock

Theoretically, thermal energy is released into the bedrock by earth currents by way of ohmic dissipation. However, this has an insignificant impact on the bedrock temperature.

Groundwater flow

Compared to the advective flow, the electro-osmotic flow can be neglected. Thus the groundwater flow is independent of the flow of electric current through the rock mass.

Groundwater pressure

Earth currents will not affect the groundwater pressure.

Table 5-22. Direct influences of the process “earth currents” on the defined geosphere variables, and a brief description of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 5.12.7)
Temperature in bedrock	No. Not significantly.	All	–
Groundwater flow	No. Not significantly.	All	–
Groundwater pressure	No.	All	–
Gas phase flow	No.	All	–
Repository geometry	No.	All	–
Fracture and pore geometry	No.	All	–
Rock stresses	No.	All	–
Matrix minerals	No.	All	–
Fracture minerals	No. Not significantly.	All	–
Groundwater composition	Yes. Earth currents redistribute ionic solutes, colloids, etc. Tracer concentrations may be affected.	All	Earth currents may transport radionuclides from flowing fracture water to stagnant (pore) water. This is pessimistically neglected. On the whole, the effect on groundwater composition is neglected.
Gas composition	No.	All	–
Structural and stray materials	Earth currents can enhance the corrosion rate of metallic structural and stray materials (such as rock reinforcements).	All	The degradation of rock reinforcements is assumed to be quick upon repository closure, regardless of the contribution from earth currents.
Saturation	No.	All	–

Gas phase flow

The gas phase flow is independent of the flow of electric currents through the rock mass.

Repository geometry

Earth currents will not affect the repository geometry (unless indirectly by corrosion of rock reinforcements, potentially leading to rock fallout).

Fracture and pore geometry

Earth currents will not affect the fracture and pore geometry.

Rock stresses

Earth currents will not affect rock stresses.

Matrix minerals

Earth currents will not affect the matrix minerals, unless they promote electrochemical reactions. However, such reactions are normally associated with ore bodies, which should be rare in the Forsmark area.

Fracture minerals

Earth currents will not affect the fracture minerals, unless they promote electrochemical reactions. Pyrite is known to take part in electrochemical reactions but the abundance of pyrite is low at the Forsmark site (Löfgren and Sidborn 2010). This is not expected to have implications for repository safety.

Groundwater composition

Earth currents are mainly propagated by ionic solutes (unless the electric field is alternating at a high frequency). This leads to a redistribution of these solutes, which may affect the water composition. This may have implications for radionuclides transported from the repository in fracture water. Normally, these radionuclides are assumed to diffuse into the microporous system of the rock matrix. If adding an electrical potential gradient over the fracture/rock matrix interface, the radionuclides will (also) electromigrate into the rock matrix. This is explained well by the Maxwell–Stefan diffusion theory (see Section 5.3). In short, the driving force for the transport is the chemical potential gradient, to which both the concentration gradient and electrical potential gradient contribute. However, as discussed in Section 5.12.1, the contribution from the electrical potential gradient is moderate to small.

For ionic solutes in terms of main constituents normally existing in the groundwater, they will exist in both the pore water and in the fracture water, and earth currents will not significantly alter how they are distributed, or their abundance. The exception is if earth currents promote electrochemical reactions that release ions that are not normally present in the groundwater. However, this is not expected at the Forsmark site.

Earth currents may also redistribute colloids and macromolecules in the fracture system. However, this is subordinate to redistribution by advection. It is conceivable that electrophoresis redistributes colloids and large size complexes from the flow path to stagnant fracture water.

Gas composition

Earth currents will not affect the gas composition.

Structural and stray materials

Earth currents can enhance the corrosion rate of structural and stray materials. Such structural and stray material would predominantly have to be metallic in nature. An example of such a material is rock reinforcements. Generally speaking, enhanced corrosion of metallic materials has been observed at the Forsmark site (Nissen et al. 2005).

Saturation

Earth currents will not affect the degree of saturation.

5.12.3 Boundary conditions

The relevant boundary conditions are the electrical potential gradients caused by anthropogenic activities, presently at the surface. As long as these potential gradients do not increase significantly, earth currents should be of little consequence for repository safety. Should they increase within reasonable bounds, the discussed processes in the geosphere should not jeopardise repository safety.

For the SFR site, which is presently covered by the Baltic Sea, one could argue that most electric current from the Fenno-Skan HVDC transmission and other anthropogenic activity would be propagated in the seawater, which would therefore shield the host rock from extensive electrical potential gradients. Therefore, one can see the presence of the overlying seawater as a boundary condition.

5.12.4 Model studies/experimental studies

In the Forsmark site investigation for the KBS-3 repository, electrical potential gradients at a few hundred metres depth at the target area have been measured and compared with the power output of the HVDC cable (Nissen et al. 2005). In the site investigations the term self-potential is used for the “natural” electrical potential of the rock, as measured with a tool that does not induce an electric field (however, in Forsmark this natural potential is affected by the HVDC power output and other anthropogenic activity). The results show that the self-potential of the rock below 100 m depth is clearly affected by the HVDC power output, and that local self-potential gradients can be significant (no measurements were performed at shallower depth). The obtained self-potential gradients, as measured over a distance of 1.5 m in packed-off boreholes, were in the range of about 10 to 100 mV/m (cf. Nissen et al. 2005, Figure 5-3 and Appendix 2).

In the site investigations for the KBS-3 repository (e.g. Nielsen and Ringgaard 2007), the self-potential has routinely been measured in open boreholes (as oppose to packed-off boreholes) in the geophysical programme. The open borehole functions as a conductor homogenising the electric field, and as a result, the large self-potential gradients measured when packing off the borehole are not seen. The reported results from these measurements are self-potentials, and not potential gradients. However, when studying data points at a distance of about 5 metres apart (chosen because this is the scale of a copper canister in the KBS-3 repository), typical self-potential gradients on the order of 10 mV/m or less can be extracted (cf. Nielsen and Ringgaard 2007, Appendices 1 and 2). Occasionally, gradients up to 50 mV/m are seen.

By comparing self-potentials in boreholes hundreds of metres from each other, large-scale potential gradients can be estimated. In this case, the effect from the open borehole functioning as a conductor is less significant. Nissen et al. (2005) report measurements of self-potentials in boreholes KFM01A and KFM04A. The distance between the boreholes is about 600 m. At KBS-3 repository depth (~500 m), the measured self-potentials in these boreholes differed by about 1 V (cf. Nissen et al. 2005, Appendix 1) resulting in a potential gradient on the order of 1 mV/m. It should be noted that these measurements were not necessarily performed at the same power output from the HVDC cable, which may affect the estimated gradient. In the surroundings of Forsmark, the (large-scale) potential gradient is believed to be around 300 mV/km (Nissen et al. 2005).

Studies of electromigration of dissolved tracers through granitic rock have been performed in the laboratory by Löfgren (2004), Löfgren and Neretnieks (2006), Löfgren et al. (2009) and Vecernik et al. (2012). In these studies a high electrical potential gradient has been used (on the order of hundreds of V/m). At such high electrical potential gradients, electromigration clearly outweighs diffusion as the most prominent transport mechanism. However, at electrical potential gradients expected in situ, diffusion is through to be roughly equal to, or outweigh, electromigration (see discussion in Section 5.12.1). In Löfgren and Neretnieks (2006) the electro-osmotic flux through granitic rock was examined. It was found to be considerably smaller than the electro-migratory flux.

5.12.5 Natural analogues/observations in nature

There are a number of observations in nature (if including railways, pipelines, power lines etc as part of nature) concerning the effect of earth currents in terms of corrosion. For an overview, see Lanzerotti and Gregori (1986) and SKB (2010e). To the knowledge of the author, no observation in nature concerning solute or colloidal transport has been directly linked to earth currents, except for measurements and experiments such as those described in Section 5.12.4).

5.12.6 Time perspective

If at all relevant, only direct earth currents induced by anthropogenic activity such as electric power production and transmission are large enough in magnitude to be of interest for SR-PSU. Such anthropogenic activity is expected to exist in the short time perspective, but is not expected to exist as the site is covered by an ice sheet during the glacial period, or submerged following the deglaciation. It is impossible to speculate on what anthropogenic activity will induce earth currents during the coming temperate and periglacial climate periods. If needed, such future anthropogenic activity could only be handled through setting up different scenarios.

5.12.7 Handling in safety assessment

In this section, the SR-PSU team gives a description of how the process is handled. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 5-21 and Table 5-22 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

Earth currents induced by anthropogenic activity are expected during this time period. However, during the excavation and operation phase there is no release of radionuclides into the geosphere. This generally also holds true for the re-saturation period as the hydraulic gradient is expected to be towards the repository.

Periods of the temperate climate domain

During the initial few hundred years, the rock support is expected to quickly corrode with rock fallout as a possible consequence.

Radionuclide release to the geosphere is expected during temperate periods. Based on the discussion in Section 5.12.1; out of the processes electromigration, electrophoresis, and electro-osmosis, it is electromigration that is judged to have the largest consequence for radionuclide transport and retention. In the experiments performed by Löfgren and Neretnieks (2006) the electro-migratory flux was compared with the diffusive flux in granitic rock. With a potential gradient of about 330 V/m, the steady state electro-migratory flux should be about 1,500 times larger than the steady state diffusive flux. Similar experiments have been performed by Löfgren et al. (2009) on rock samples from the Forsmark site, and with pore water salinities resembling those at the site.

In the following back of the envelope assessment it is examined what the result would be if rescaling this experimental potential gradient to that expected in situ. Here the in situ electrical potential gradient is assumed to be 50 mV/m, based on the in situ measurements by Nissen et al. (2005). It should be noted that this gradient is not based on measurements in the SFR host rock, which is possibly shielded by the Baltic Sea. If anyhow assuming this rather large potential gradient, the electro-migratory flux through the rock sample would be about one fourth[11] of the diffusive flux. Making such a back of the envelope calculation has a number of flaws. For one, it is uncertain if the scaling is linear over this large range of electrical potential gradients in crystalline rock. Also, the scale dependence of electromigration is different from that of diffusion. If summarising the dependence of sample length, at short penetration depths, diffusion would even more outweigh electromigration, while at very large penetration depths, the situation would be reversed. Therefore, electromigration is likely more important for non-sorbing solutes than for sorbing. With this in mind, one can still make the statement that the electro-migratory flux should be roughly on the same order of magnitude as the diffusive flux in the SFR host rock, or in many cases lower.

As electromigration supports matrix diffusion in retarding radionuclides in the geosphere, it has been decided to pessimistically disregard the process in SR-PSU. With this decision in mind, the shortcomings in the above described back of the envelope assessment are accepted. As electromigration of radionuclides is judged to be the most prominent process associated with earth currents; earth currents all together are neglected in SR-PSU radionuclide modelling.

Periods of periglacial climate domain

Prior to the first periglacial period, (metallic) rock reinforcements are expected to have been degraded. Earth currents are neglected in radionuclide transport modelling for these periods, based on the same reasoning as for periods of the temperate climate domain.

Glacial climate domain

Anthropogenic activity giving rise to earth currents is unlikely during these periods, due to the presence of the ice sheet.

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[11] Calculated by inserting the electrical potential gradient 50 mV/m in Equation 7 in Löfgren and Neretnieks (2006), applied to a 12 cm long sample.

Earthquakes

No relation between earthquakes and earth currents has been identified, except for momentarily effects in conjunction to the short period of time when the earthquake is active (as the rock movement could induce piezoelectric effects). Such momentarily effects on earth currents are inconsequential for repository safety.

Handling relative to geosphere variables

Temperature in bedrock

The energy induced into the host rock by earth currents has an insignificant effect on the rock temperature and is neglected.

Groundwater flow

The effect that an electro-osmotic flow has on the advective flow in the fracture system is insignificant and is neglected.

Groundwater pressure

Changes in groundwater pressure will not change the impact of earth currents on the safety assessment, and has been neglected.

Gas phase flow

No dependency between gas phase flow and earth currents exists. In this statement, the potential impact of earth currents on gas production from foreign materials in the repository vaults has not been taken into account.

Repository geometry

In the back of the envelope assessment described above, resulting in the judgment that that earth currents can be neglected; the repository geometry was not taken into account. If the repository affects the electric field in the surrounding host rock, the effect would likely be limited to the host rock close to the underground openings.

Fracture and pore geometry

The fracture and pore geometry of the host rock at the Forsmark site has been taken into account when making the back of the envelope assessment described above, as it is based on results from experiments carried out on site specific rock samples. Also, the impact of water-bearing fractures on electric currents propagated in the rock mass has been assessed based on site specific information (e.g. Löfgren and Neretnieks 2005, Löfgren 2014).

Rock stresses

Changes in rock stresses may affect the electric current running through the rock (e.g. Skagius and Neretnieks 1986). However, this is judged to have a very small impact on the magnitude of earth currents and an insignificant impact on repository safety.

Matrix minerals

The host rock at the Forsmark site, which generally lacks in ore bodies, has been taken into account in making the assessment that earth currents will not significantly affect the radionuclide transport and retention. The impact of the part of earth currents propagated in the diffuse double layer, at the charged mineral surfaces in the rock matrix, has been assessed based on experimental data from site specific rock. This impact may possibly increase the electromigration of weekly sorbing cations into the rock matrix thereby increasing the retention capacity of the rock matrix. However, this is neglected in SR-PSU.

Fracture minerals

Fracture minerals at the Forsmark site exist in too small a volume to be of consequence for earth currents.

Groundwater composition

It is judged that earth currents will not affect the general groundwater chemistry, in terms the groundwater main constituents. However, they may affect the distribution of tracer elements (e.g. radionuclides) between the fracture water and pore water of the rock matrix. The process that is judged to have the greatest effect on this redistribution is electromigration. Even though the process would, to some extent, increase the migration of radionuclides and other tracers from the fracture water to the pore water (or vice versa), it is judged that this process should be pessimistically neglected in SR-PSU.

Gas composition

No direct dependency between gas composition and earth currents exists.

Saturation

The host rock is assumed to be fully saturated at the relevant time periods in SR-PSU.

5.12.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Experiments designed to investigate the electro-migratory flux in the granitic rock matrix have been performed at very high electrical potential gradients (e.g. Löfgren and Neretnieks 2006). It is therefore uncertain if the results can be extrapolated to the electrical potential gradients expected in situ.

There are some remaining issues concerning the transport of solutes in the electrical double layer of mineral grains (see also Section 5.3). The uncertainties in mechanistic understanding concerning multicomponent transport, discussed in Section 5.3, also apply for electro-migratory transport.

Furthermore, which could also be viewed upon as data uncertainty, there is a lack of reliable measurement data concerning the electrical potential gradient at different scales at the Forsmark site at depth (especially at the SFR site).

Model simplification uncertainties

No modelling is performed with the aim at simulating earth currents. Accordingly, no model simplification uncertainties exist. There are substantial simplifications in the back of the envelope calculation presented above, comparing diffusion and electromigration, and therefore the result should be used with great care.

5.12.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

6 Radionuclide transport processes

6.1 Speciation of radionuclides

When one or more dissolved solutes react to form a compound where the individual constituents are held together by chemical bonds rather than by electrostatic forces, the product is termed a *complex*. When discussing the complexation reaction of a specific solute, the dissolved species with which it reacts is commonly referred to as a *ligand*. The free concentration of a solute makes up a variable part of, what is referred to as, the *total dissolved concentration* of a substance. The distribution of a particular solute amongst various complex forms (termed *species*), whether it be a nuclide or a major groundwater component, is referred to as the *speciation* of that solute. Speciation also can refer to the particular redox state of an element amongst various redox states in which it can reside (i.e. *redox speciation*). The redox state of a solution is defined relative to other redox pairs.

Surface complexation is analogous to aqueous phase complexation with the exception that one of the ligands takes the form of a reactive functional group on a mineral surface in the case of surface complexation and the resulting complex is therefore immobile (unless the surface itself is mobile such as in the case of a carrier colloid particle). The formation of aqueous complexes may greatly affect the distribution of a radionuclide between the aqueous and solid phases both directly and indirectly. Knowledge of the speciation of a nuclide is therefore very useful for understanding the impact that altered physicochemical conditions such as a change in pH, temperature, or gas partial pressure might have upon the mobility of that nuclide in flowing groundwater. Knowing the relative predominance of different complexed forms has also proven useful in the past for selection of surface reactions used to represent a sorption process in modelling (e.g. Bradbury and Baeyens 2009).

6.1.1 Overview/general description

Speciation can affect the mobility of a nuclide by binding the nuclide in a relatively stable, less-reactive form. In Crawford (2010), this was considered to be an indirect competitive binding effect. The competition of various dissolved solutes for a limited number of surface binding sites, on the other hand was deemed to be a direct competitive effect in this previous work. Speciation may also have second-order indirect effects by way of an intermediary process that influences the speciation of a different groundwater solute which, in turn, conveys an influence on the sorption process of interest. Effects of speciation where dissolved ligands bind with nuclides thereby reducing their sorptivity are generally well-known and understood. Other indirect influences of a second-order nature have often more subtle interdependencies and are more easily overlooked in groundwater modelling.

Two key groundwater compositional variables that have strong influences on sorptivity are pH and carbonate concentration, under the chemical conditions prevailing at SFR. The pH can influence the proportion of surface reactive sites available for binding of the nuclide (a direct effect) or it may promote hydrolysis reactions of the nuclide in the aqueous phase, thereby sequestering it amongst various hydroxyl-complex forms in the solution (an indirect, competitive effect). The carbonate concentration may also have an indirect effect on sorption through binding the nuclide in carbonate complex forms in solution. The pH, however, can also influence the speciation of the dissolved carbonate and thus the availability of the particular carbonate ligand with which the nuclide reacts. This might be regarded as a second-order effect of pH since it indirectly influences the sorption of the nuclide by way of secondary reactions involving carbonate speciation.

Other second-order indirect effects can also occur, for example, in the case where speciation effects increase or decrease the availability of a solute that would normally compete for sorption sites with a migrating nuclide (or, alters the availability of a ligand that would otherwise strongly bind the nuclide in aqueous solution). One example of this is the sorption of Ni^{2+}. Although Ni is not known to be a redox sensitive nuclide, its sorption may be influenced by competition for binding sites with dissolved Fe^{2+}. Since Fe^{2+} can exist in significantly elevated concentrations under reducing conditions relative to that typically found under oxidising conditions, the sorption of Ni^{2+} may be indirectly impacted by the redox state of the groundwater.

It is noted here, however, that it is sometimes unnecessarily confusing to strictly categorise the influence as having a direct or indirect impact on sorption, since the definition is arbitrary and it is sufficient to simply note that the totality of these effects needs to be considered in modelling of radionuclide migration. Since the coupled dependencies between different groundwater compositional variables give rise to non-linear effects, it is generally necessary to model all of these interactions simultaneously and it is difficult to draw quantitative conclusion from consideration of any individual process in isolation.

As a simple example, it is useful to consider the impact of carbonate complexation on a relatively well-behaved solute such as Am^{3+}. At a typical groundwater pH of 8.5, for example, the free concentration of dissolved Am^{3+} may be as little as 0.1%, or less of the total Am concentration which, is likely to be dominated by carbonated complexed forms in a non-saline groundwater. Since it is the free Am^{3+} species that reacts to form surface complexes with hydroxyl-surface reactive groups, one might suspect that the sorptivity of Am would be reduced by at least 3 orders of magnitude relative to that obtained in the absence of carbonate complexation reactions involving Am^{3+}. This, however, is generally not the case and any reduction in sorptivity due to binding of Am in the solution phase is far less than what one would naively predict on the basis of speciation considerations. The situation can be further complicated (although this is neglected in the current hypothetical example) in that sorption reactions involving ternary surface complexation reactions involving nuclides and dissolved carbonate with surface hydroxyl groups can also occur if the carbonate concentration is sufficiently high (e.g. Marques Fernandes et al. 2010).

The reason for this discrepancy is that the speciation of the aqueous phase cannot be considered in isolation of the surface reactions involving Am since the distribution of Am in the system dynamically shifts in response to changes in any part of the coupled reactive system. In fact, the only situation in which the binding of a nuclide in an aqueous complex could conceivably have this direct and proportional effect on sorptivity would be in the case of an effectively irreversible reaction (for example, with an exceptionally strong complexing agent). In the Am example, discussed here the moment the free concentration of Am^{3+} is depleted by reaction to form a surface complex, some of the carbonate complexed inventory would react to replenish the free concentration and thereby re-establish the equilibrium proportions of speciated forms in the aqueous phase.

Such reasoning can also be applied to redox sensitive nuclides. In this case, aqueous speciation calculations are often used to make prognostications whether the nuclide should be present in an oxidised or reduced form with resultant implications for nuclide mobility (given that oxidised species are frequently more mobile). Under certain conditions it is possible for the coupled reactions to give rise to a situation whereby the predominant redox form in solution differs from the predominant redox form of the sorbed fraction. This is, of course, complicated by kinetic effects involving transformation of one redox state to another (since redox systems in nature are frequently in a state of disequilibrium), although in the equilibrium description of the system it is perfectly reasonable and internally consistent with the underlying mathematical formalism describing the speciation.

6.1.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 6-3 outlines how the process is influenced by the defined geosphere variables, while Table 6-4 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. In Section 6.1.7, this handling is further detailed in a discussion provided by the SR-PSU team.

Table 6-1. Direct influences of defined geosphere variables on the process "speciation of radionuclides" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 6.1.7)
Temperature in bedrock	Yes, temperature influences thermodynamics of chemical reactions.	T/P/G	Partially considered. In reaction calculations an in situ temperature of 15°C is assumed as a calculation basis. Accuracy of extrapolation from 25°C reference is dependent on completeness of thermodynamic database.
Groundwater flow	No, but indirectly since the rate of flow through and around repository is coupled to the impact of OPC leachate on groundwater compositional variables (high pH plume).	T/P/G	Speciation and sorption calculations in support of K_d recommendations assume pH buffering by hydrodynamic mixing of type groundwaters with a simplified OPC leachate giving a span of groundwater compositions dependent on the equivalent mixing fraction of OPC leachate in flow pathlines leaving the repository.
Groundwater pressure	Yes, pressure influences thermodynamics of chemical reactions.	T/P/G	Not considered on account of the effects being minor at the depth considered. Accuracy of extrapolation from 1 atm is dependent on completeness of thermodynamic database.
Gas phase flow	No, but indirectly exchange of volatile components (e.g. CO_2, O_2, H_2S, CH_4 etc.) in the presence of a gas phase can influence inventory of dissolved components and thus speciation.	T/P/G	Indirectly considered by way of hypothetical partial pressure of volatiles in equilibrium with groundwater composition. No scenarios considered for free-phase gas flow however.
Repository geometry	No, but indirectly by way of the impact of repository geometry on groundwater flow and OPC leachate generation.	T/P/G	Not considered in calculations.
Fracture and pore geometry	No, but indirectly by way of channelling effects and influence on hydrodynamic mixing processes.	T/P/G	Not considered in calculations.
Rock stresses	No, but indirectly through impact of contact stresses on mineral dissolution/precipitation.	T/P/G	Not considered in calculations (effect is deemed miniscule).
Matrix minerals	No, but indirectly exchange of groundwater solutes with matrix minerals by dissolution/precipitation and ion-exchange has strong impact on speciation.	T/P/G	Not directly considered since already handled in definition of type groundwater compositions delivered by the hydrochemical characterisation.
Fracture minerals	No, but indirectly exchange of groundwater solutes with fracture minerals by dissolution/precipitation and ion-exchange has strong impact on speciation.	T/P/G	Considered in reaction calculations made in support of K_d recommendations.
Groundwater composition	Yes.	T/P/G	Considered in reaction calculations made in support of K_d recommendations.
Gas composition	No, but indirectly by influencing water composition through dissolution of gas.	T/P/G	Indirectly considered by way of hypothetical partial pressure of volatiles in equilibrium with groundwater composition.
Structural and stray materials	No, but indirectly via groundwater composition since presence and type of structural material in contact with groundwater has impact on OPC leachate.	T/P/G	Indirectly considered in reaction calculations made in support of K_d recommendations by way of hypothetical pH buffering of OPC leachate.
Saturation	No, but indirectly.	T/P/G	Not considered directly, but degree of saturation is coupled to presence of gas phase as discussed above which also influences redox speciation.

Explanation of Table 6-1

Temperature in bedrock

Thermodynamic data given in thermodynamic databases are compiled for a reference temperature of 25°C and 1 atm pressure. Temperature has an impact on chemical reactions by way of altering the equilibrium constant for the reaction. As a general rule of thumb, reactions which are endothermic (i.e. the forward reaction consumes heat) are favoured by increasing temperatures and diminished by reduced temperatures. Reactions which are exothermic (i.e. the forward reaction produces heat) are diminished by increasing temperatures and favoured by decreasing temperatures. The effect is quantified in speciation calculations by adjustment of equilibrium constants from the reference temperature to the temperature of interest using the Van't Hoff equation (e.g. Langmuir 1997) or analytical expressions. For the purposes of recommending K_d data for use in SR-PSU an average in situ temperature of 15°C has been assumed to be approximately representative for all groundwater time domains. The impact of temperature is only partially accounted for, however, since reaction enthalpy data for all relevant groundwater reactions is generally not available in the SKB thermodynamic database (Duro et al. 2006) nor others in common use. For the small temperature deviations as considered here, however, only very small differences in calculated speciation is expected relative to 25°C and the impact of temperature may be considered to be very minor.

Groundwater flow

Groundwater flow is not directly considered in radionuclide speciation calculations for the geosphere. Its impact appears indirectly, however, through the assumption of hydrodynamic mixing giving rise to the pH buffering processes assumed to occur in the geosphere along migration paths leading from the repository to the biosphere.

Groundwater pressure

Groundwater pressure is not considered in the speciation calculations. This is due to the fact that it is not considered to have a significant effect on the processes modelled in the relevant depth range and due to a lack of relevant data to perform such calculations on the full suite of chemical reactions likely to occur in groundwater.

Gas phase flow

Gas phase flow is not directly considered in radionuclide speciation calculations on account of the absence of a relevant scenario defined for such a process in the geosphere. The impact of gas phase exchange of reactive components with the groundwater is only indirectly considered by way of the hypothetical equivalent partial pressure of various gas components (principally CO_2 and O_2) obtained in reaction calculations.

Repository geometry

Repository geometry is not considered in the radionuclide speciation calculations although it is known to have an effect on the rate of OPC leachate release to the geosphere flowpaths and thus will have an impact on the potential development of a high pH plume. Rather, hypothetical mixing calculations of a more general nature have been considered for the assessment of radionuclide speciation where prevailing groundwater types for different climatic domains are mixed with a range of OPC leachate fractions (ranging from 0%–100% OPC).

Fracture and pore geometry

Fracture and pore geometry is not considered in the radionuclide speciation calculations although they may have an effect on channelling and consequently, the extent of hydrodynamic mixing along geosphere flowpaths. The dynamics of hydrodynamic mixing thus has an impact on the spatial extent and rate of mitigation of a potential high pH plume.

Rock stresses

Rock stresses are not considered in the radionuclide speciation calculations.

Matrix minerals

Matrix minerals are not directly considered in the radionuclide speciation reactions on account of them already being considered in the composition of "type" groundwaters for the different time domains of the safety assessment as delivered by the hydrochemical characterisation programme as an input.

Fracture minerals

Precipitation-dissolution processes involving fracture minerals are considered in the mixing calculations underlying the radionuclide speciation and sorption simulations.

Groundwater composition

Groundwater composition is considered both directly in speciation and sorption calculations as well as in the mixing calculations describing the buffering of groundwater chemistry in response to mixing with OPC leachate along migration paths in the geosphere.

Gas composition

Gas composition is not directly considered in radionuclide speciation calculations. The impact of gas phase exchange of reactive components with the groundwater is only indirectly considered by way of the hypothetical equivalent partial pressure of various gas components (principally CO_2 and O_2) obtained in reaction calculations.

Structural and stray materials

The existence of structural and stray materials is not considered in the radionuclide speciation calculations although it is known to have an effect on both the rate of OPC leachate release to the geosphere flowpaths and its composition. In the simplified speciation and sorption calculations which have been made in support of the K_d recommendation, the composition of an OPC-like leachate end-member is approximated by assuming portlandite equilibrium with the prevailing "type" groundwater comprising the opposite end-member in binary mixing calculations.

Saturation

Saturation is not directly considered in radionuclide speciation calculations. The impact of gas phase exchange of reactive components with the groundwater is only indirectly considered by way of the hypothetical equivalent partial pressure of various gas components (principally CO_2 and O_2) obtained in reaction calculations.

Explanation of Table 6-2

Temperature in bedrock

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the energy balance of the groundwater–rock system, and thus will not affect the bedrock temperature.

Groundwater flow

The effect of radionuclide speciation on groundwater composition (thus also water viscosity and density) is too small to affect the groundwater flow in any significant way.

Groundwater pressure

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the groundwater pressure.

Table 6-2. Direct influences of the process "speciation of radionuclides" on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 6.1.7)
Temperature in bedrock	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence temperature of bedrock.	All	
Groundwater flow	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence groundwater flow.	All	
Groundwater pressure	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence groundwater pressure.	All	
Gas phase flow	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence gas phase flow.	All	
Repository geometry	No. No relevant interaction exists.	All	
Fracture and pore geometry	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence fracture and pore geometry.	All	
Rock stresses	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence rock stresses.	All	
Matrix minerals	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence abundance or reactivity of matrix minerals.	All	
Fracture minerals	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence abundance or reactivity of fracture minerals.	All	
Groundwater composition	No effect on bulk composition, although speciation of radionuclide will have an impact on the total concentration of that nuclide (and possibly that of radionuclides competing for the same sorption binding sites).	All	Considered for the recommendation of K_d values for radionuclide transport calculations.
Gas composition	No. Speciation of radionuclides at the very low concentrations expected is not deemed to influence bulk gas phase composition.	All	
Structural and stray materials	No. No relevant interaction exists.	All	
Saturation	No. No relevant interaction exists.	All	

Gas phase flow

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the flow or bulk composition of any gas phases present.

Repository geometry

Speciation of radionuclides does not have any relevant influence on the repository geometry.

Fracture and pore geometry

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the geometry of fractures or pore-apertures in any significant way.

Rock stresses

Speciation of radionuclides is not expected to affect the stress situation of the bedrock.

Matrix minerals

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the matrix physical or chemical properties in any significant way.

Fracture minerals

Speciation of radionuclides at the concentration levels envisaged is not expected to affect reactive properties of the fracture minerals in any significant way.

Groundwater composition

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the bulk groundwater composition (here taken to include redox), although it will exert an influence on the total amount of that radionuclide present in the groundwater.

Gas composition

Speciation of radionuclides at the concentration levels envisaged is not expected to affect the bulk gas phase composition.

Structural and stray materials

Speciation of radionuclides does not have any relevant influence on structural and stray materials.

Saturation

Speciation of radionuclides is not expected to affect the degree of saturation in any significant way.

6.1.3 Boundary conditions

Speciation of radionuclides at the concentration levels envisaged is a small scale process that has an essentially one-way dependency on groundwater composition. The concentrations of transported radionuclides are deemed to be far too low to have any discernible impact on bulk groundwater composition or geosphere mineralogy. The groundwater composition both determines the speciation of the transported radionuclide and the protonation–deprotonation state of reactive groups at the solid-liquid interface. For example, the pH determines whether the fracture mineral hematite is positively or negatively charged, and therefore the preference for cationic or anionic sorption. Aqueous phase speciation reactions are also governed by the intensive variables temperature and pressure, although the effect is relatively minor (particularly so, for pressure effects) in the temperature and pressure ranges considered.

6.1.4 Model studies/experimental studies

Radionuclide speciation in environmental settings has been studied extensively and is extremely well-documented in the open literature. The state of the art concerning radionuclide speciation has been summarised in 10 reports published within the OECD-NEA Thermochemical Database (TDB) project. The thermodynamic modelling database used by SKB (Duro et al. 2006) builds largely upon data contained in the OECD-NEA chemical thermodynamics series of reports and the reviews of thermodynamic data documented therein.

6.1.5 Natural analogues/observations in nature

Chemical speciation of radionuclides in natural environmental settings is a fundamental aspect of their aquatic chemistry that is well characterised and documented in the open literature. The review articles by Bruno et al. (2002), Choppin and Stout (1989), Choppin (2003) and Clark et al. (1995) and references therein provide a good background with specific focus on chemical speciation of actinides in the context of radioactive waste management. Many other naturally occurring and anthropogenic isotopes have applications as tracer substances in hydrogeology and paleoclimatology and are well described (see e.g. Clark and Fritz 1997, Fairchild et al. 2006). Speciation of radionuclides has also been examined in a number of natural analogue studies (for a detailed account, see Miller et al. 2000).

6.1.6 Time perspective

Speciation of radionuclides is an important aspect of their chemical reactivity with strong relevance for their mobility during all time domains considered in the SR-PSU safety assessment.

6.1.7 Handling in safety assessment

In this section, the SR-PSU team gives recommendations on how to handle the process of radionuclide speciation. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Section 6.1.2 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

During the excavation/operation phase, aerated waters could be expected to flow in fractures in the vicinity of the tunnels and engineered structures. The presence of an extensive gas phase (air) in the various unsaturated compartments of the repository system may be expected to have some influence on groundwater that it comes in direct contact with. The changes in the groundwater chemistry that this entails may be expected to have an impact on radionuclide speciation, although radionuclides are not expected to be released during this phase of the repository operation.

Temperate climate domain

During the temperate climate period the groundwater is expected to be of a somewhat saline character with relatively higher concentrations of base cations, chloride and sulphate although lower concentrations of carbonate than for a groundwater of more meteoric/fresh character. Radionuclides that sorb by ion-exchange typically exhibit weaker sorption under saline conditions due largely to increased competition for cation exchange sites with Ca^{2+} and Na^{+}, although a number of the surface complexing nuclides that are affected by carbonate complexation exhibit stronger sorption. The groundwater during this time domain is expected to be relatively reducing at –100 mV to –350 mV favouring the predominance of the relatively more strongly sorbing, reduced states of the main redox sensitive nuclides, i.e. U(IV), Np(IV), Pu(III/IV), and Tc(IV). The composition of the groundwater and its impact on speciation during this time domain is specifically considered in detail for the recommendation of K_d values for geosphere transport calculations wherever it is feasible to do so.

Periglacial climate domain

During the Periglacial climate domain, the groundwater is more meteoric in character with a concentration of base cations, chloride, and sulphate roughly 2 orders of magnitude lower than under the Temperate climate domain discussed above. The dissolved carbonate concentration is roughly 3–5 times higher than that characteristic of the more saline Temperate groundwater. Radionuclides that sorb by ion-exchange have relatively stronger sorption under these more dilute conditions due to lessened competition for cation exchange sites with Ca^{2+} and Na^{+}, although a number of the surface complexing nuclides that are affected by carbonate complexation exhibit weaker sorption owing to competition to bind nuclides in aqueous complexed forms. The groundwater during this time domain is expected to be relatively reducing at –135 mV to –300 mV favouring the predominance of the relatively more strongly sorbing, reduced states of the main redox sensitive nuclides, i.e. U(IV), Np(IV), Pu(III/IV), and Tc(IV). The composition of the groundwater and its impact on speciation during this time domain is specifically considered in detail for the recommendation of K_d values for geosphere transport calculations wherever it is feasible to do so.

Glacial climate domain

The Glacial climate domain is characterised by a groundwater with a much more dilute character and an elevated pH of 9.3 relative to the typical groundwater types existing during the other climate domains. Concentrations of the main base cations, chloride, and sulphate are reduced by at least 2 orders of magnitude relative to the Periglacial climate domain (~4 orders of magnitude relative to the Temperate domain). The dissolved carbonate concentration is much less than for the other typical groundwater types during the Temperate or Periglacial climate domains, although it is sufficiently high to make it the most important aqueous anion. The groundwater is expected to be poorly poised owing to the low concentrations of dissolved species giving a low redox buffering capacity. A typical groundwater is expected to be relatively oxidising with an average Eh of +400 mV, although this could range from as little as –290 mV to +900 mV. The average groundwater is sufficiently oxidising that the predominance of the more strongly sorbing reduced states of the redox sensitive nuclides cannot be guaranteed. During this time domain it is more likely that the U(VI), Np(V), and Tc(IV) states are predominant, although Pu(IV) is still expected to be the main Pu redox species.

Earthquakes

Earthquakes are not expected to have any direct influence on radionuclide speciation.

Handling relative to geosphere variables

Temperature in bedrock

The effect of temperature is specifically accounted for in the radionuclide speciation and sorption modelling calculations used in support of the K_d recommendations. An average in situ groundwater temperature of 15°C is assumed as a basis for calculations in all time domains.

Groundwater flow

Groundwater flow is not expected to have any direct influence on radionuclide speciation except for the impact that it has on the extent of hydrodynamic mixing and the formation of a plume of OPC leachate affected groundwater. The possibility of an OPC plume is considered in the recommendation of K_d values wherever deemed appropriate to do so.

Groundwater pressure

Groundwater pressure is not considered in radionuclide speciation calculations since its effect is expected to be very small at the depth ranges considered.

Gas phase flow

Gas phase flow is not considered in radionuclide speciation calculations.

Repository geometry

Repository geometry is not considered in radionuclide speciation calculations.

Fracture and pore geometry

Fracture and pore geometry is not considered in radionuclide speciation calculations.

Rock stresses

Rock stresses are not considered in radionuclide speciation calculations.

Matrix minerals

Primary matrix mineralogy is not considered directly in radionuclide speciation calculations, although it appears implicitly by way of underlying assumptions in the groundwater compositions used as input data to the K_d recommendation. Secondary minerals such as calcite, hydrous ferric oxide, and apatite are, however, considered in the radionuclide speciation calculations.

Fracture minerals

Fracture minerals are considered in radionuclide speciation calculations to the extent that calcite residing in fractures is assumed to dissolve and precipitate to buffer concentrations of dissolved carbonate in the modelling of groundwater composition. The mineral apatite is also assumed to be present in fracture coatings and equilibrium with this mineral is assumed to fix dissolved concentrations of phosphate in radionuclide speciation calculations.

Groundwater composition

Groundwater composition has a direct impact on radionuclide speciation by way of the dissolved concentrations of various ligands which form aqueous phase complexes with radionuclides. The chemical composition of groundwater is considered in the radionuclide speciation and sorption modelling calculations used in support of the K_d recommendations.

Gas composition

Gas composition is not considered directly in radionuclide speciation calculations, although it appears indirectly by way of the hypothetical equivalent partial pressure of various gas components (principally CO_2 and O_2) in equilibrium with specified groundwater compositions.

Structural and stray materials

Structural and stray materials are considered in radionuclide speciation calculations to the extent that they may release high pH leachate which may have an impact on groundwater composition. This is handled in radionuclide speciation calculations by consideration of a range of mixing fractions of a simplified OPC leachate (portlandite equilibrated groundwater) with unaffected groundwater, although without direct consideration of the materials from which the leachate originates.

Saturation

The geosphere system is considered to be fully saturated for the purposes of radionuclide speciation calculations.

6.1.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Although the general principles underlying radionuclide speciation modelling are well understood there are a number of remaining uncertainties which affect the ability of modelling to correctly predict the speciation of radionuclides under differing groundwater chemical conditions. Chief among these is the completeness and internal consistency of thermodynamic databases used to model the relevant reactive processes. In some cases, important chemical reactions may be absent if the application focus area of the database is different to that for which it is being used. In the SKB thermodynamic database (SKB-TDB), for example, the element Cd only appears in reactions pertinent to the speciation of Se oxyanions in storage canisters for spent nuclear fuel, other reactions relating to the speciation of Cd^{2+} being notably absent. If the database is to be used to simulate Cd^{2+} speciation in the geosphere then missing reactions must be considered and included in the calculations. On account of the very short half-life of ^{113m}Cd, however, this is not considered a deficiency for the present example since this radioelement will only be important in scenarios of very fast release and its speciation therefore does not need to be considered in detail.

Another key uncertainty is the fact that many important speciation reactions may not be well characterised and have highly uncertain (or estimated) thermodynamic constants. In some cases, reactions that are suspected or known to exist are eliminated from databases since it is not possible to provide internally consistent or accurate thermodynamic constants. Some reactions may also be included in thermodynamic databases even though there is little direct spectroscopic evidence for their existence. The inclusion of such reactions in databases is predicated entirely upon hypothetical reaction mechanisms used to fit experimental data under specific chemical conditions. The use of such reactions in speciation calculations at groundwater compositions outside of their range of calibration is therefore subject to great uncertainty if the postulated species do not, in fact, exist. For the most part, however, procedures have been adopted in the selection of data within the NEA thermochemical database project and in the formulation of the derivative SKB-TDB to avoid such uncertainties to the extent that this is possible. A particular uncertainty of great import for SR-PSU is the fact that the sorptive behaviours and solubility constraining phases of many radionuclides at high pH are not well characterised (see e.g. Linklater et al. 1996). Most of the data in thermodynamic databases extrapolate from experiments made at much lower pH levels and could not be applicable at high pH conditions.

A further uncertainty, which is of some relevance for the SR-PSU calculations, is the completeness and internal consistency of reaction enthalpy data needed to simulate radionuclide speciation at temperatures other than at standard conditions (i.e. 25°C and 1 atm total pressure). Although pressure effects are neglected in SR-PSU radionuclide speciation calculations, the average groundwater temperature is assumed to be 15°C in the speciation calculations made in support of geosphere K_d selection. In this case, reaction enthalpy data are unknown for many important reactions and extrapolation to other temperatures may therefore result in a minor loss of precision and internal consistency. It is deemed, however, that the differences in the present case are sufficiently small that this can be neglected. The accuracy of the modelling results is therefore considered to be adequate and within the implied uncertainty ranges of the underlying thermodynamic data.

Any consideration of mechanistic uncertainties in radionuclide speciation modelling, however, is incomplete without consideration of the possibility of the impact of unknown unknowns. In this case, it is necessary to acknowledge the possible existence of important radionuclide speciation reactions that are either unknown or masked by other processes and erroneous reaction mechanisms assumed in modelling.

Model simplification uncertainties

Thermodynamic models used in radionuclide speciation calculations are generally very well developed and can accurately represent reality provided the underlying thermodynamic database used in calculations is complete and correct. The main non-database related modelling uncertainty encountered in the calculation of radionuclide speciation is the underlying model used to estimate aqueous phase activities. Since thermodynamic equilibria are described in terms of species activity (actually, chemical potential when considered at an even lower level of abstraction) rather than concentrations, corrections need to be introduced to calculate the concentrations of species at equilibrium. The species activity is proportional to the molality of a species although with a constant of proportionality that depends upon the ionic strength of the solution. The constant of proportionality is termed the activity coefficient.

Different models of varying complexity are used for the estimation of activity coefficients (see e.g. Langmuir 1997). These include the Debye–Hückel, Davies, Truesdell–Jones (also, variously referred to in various forms as the extended Debye–Hückel or b-dot model). These are mostly useful at low to intermediate ionic strengths (usually defined as not exceeding that of seawater). The Davies and Truesdell–Jones approaches are categorised as *specific ion interation theories* (SIT) since they include additional ion-specific parameters. For brine solutions which may be significantly more concentrated than seawater, the Pitzer model must be used. It can be noted that at low ionic strengths, results obtained using the simplified models are usually considered to be sufficiently accurate, although significant deviations appear at high ionic strengths. The more sophisticated specific ion interaction models such as Truesdell–Jones require species-specific parameters which may not be available for all relevant solutes in a reaction calculation. The Pitzer model is even more difficult to accurately parameterise since additional binary interaction coefficients are need for species interactions in concentrated solutions. Radionuclide speciation modelling at high ionic strength is therefore subject to considerable uncertainty. It can be noted that the SKB thermodynamic database (which incorporates SIT activity model parameters) is based in large part on the work carried out in the OECD NEA Thermochemical Database (TDB) project which attempts to reconcile thermodynamic and electrolyte theory in a consistent manner. The SIT activity model, however, is considered sufficiently accurate for the present application within SR-PSU and this uncertainty is deemed to be of only minor importance for the groundwater compositions under consideration.

6.1.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

6.2 Transport of radionuclides in the water phase

6.2.1 Overview/general description

A number of processes will, or could, influence the transport of radionuclides in the water phase: advective transport and mixing of dissolved species; diffusive transport in stagnant water volumes in fractures and rock matrix; sorption; colloid transport; and radioactive decay. All of these have been discussed previously in connection with processes occurring in the geosphere, or in the case of decay, in the **Waste process report**.

In this section, the integrated aspects of these processes and their handling in the safety assessment SR-PSU are discussed. The main transport processes of radionuclides and the modelling of these processes have been the focus of the EU-project RETROCK (2004, 2005) involving both implementers, including SKB, and a regulator. The approach adopted in SR-PSU and described below is based largely on the RETROCK conclusions and experience from SR-Can and SR-Site. The general description in the following paragraphs is also taken, in shortened form and modified according to SR-PSU as needed, directly from RETROCK (2005).

The dominating transport mechanism for solutes in fractured rock is with the flowing groundwater. Since water flow is restricted to the fractures, the dimensions, shape, orientation and connectivity of the fractures determine the properties of the flow paths in the rock. Very small-scale features of the fractures, such as aperture variations, may have an important influence on the flow paths. Preferential flow paths or channels may develop through parts of the fractures with larger aperture. Of special interest are fast flow channels with a very small interaction area with the rock.

The migration rate of a radionuclide is usually much lower than the velocity of water. This is due to two general retention mechanisms: first, radionuclides in the fracture network enter the internal porous network of the rock matrix by diffusion, and second, radionuclides are removed from the aqueous phase by adsorption, surface precipitation and co-precipitation, and deposited onto the mineral surfaces of the rock or fracture fillings.

The coupling between retention and flow characteristics is usually referred to as flow-related transport resistance or hydrodynamic control of retention, and is in SKB applications denoted by *F* [T/L]. It is also frequently referred to as the F-factor, or F-quotient. The important quantity is the ratio between the mass flux into the matrix and the mass flux in the flowing water. The F-factor can be defined in terms of the fluid velocity, v_i (L/T) and fracture aperture, $\delta_{t(i)}$ (L) as:

$$F = 2\int_0^{L_p} \frac{1}{v(x)\delta_t(x)}dx = 2\sum_i \frac{L_i}{v_i\delta_{t(i)}}$$ Equation 6-1

In the simplified case of a uniform fracture of width W and length L, this ratio is proportional to the area of the fracture ($2WL$ or "flow wetted surface area") divided by the groundwater flow rate Q in the fracture. For a fracture network, a summation is made over all fractures i along a flow path (or an equivalent integration of continuously variable hydrodynamic properties). The flow-related transport resistance is then given by:

$$F = 2\int_0^{L_p} \frac{W(x)}{Q(x)} dx = 2\sum_i \frac{W_i L_i}{Q_i} \qquad \text{Equation 6-2}$$

In a streamtube formulation, this might also be defined in terms of the specific flow-wetted surface, $a_{R(i)}$ (L^2/L^3) and Darcy flux, u_i (L^3/L^2T) as:

$$F = \int_0^{L_p} \frac{a_R(x)}{u(x)} dx = \sum_i \frac{a_{R(i)} L_i}{u_i} \qquad \text{Equation 6-3}$$

In the general case of heterogeneous and intersecting fractures, it can still be shown that the important entity F for the flow paths always can be determined once the flow and the geometry of the flow field are known. As outlined above, the F-factor can be defined both in terms of a summation of parameter groups for a sequence of discrete flowpath elements or an equivalent integration along a pathline of continuously variable flowpath parameters. It is noted that the physical entities comprising the above integral forms are functions of the distance along the pathline. The flow-related transport resistance is defined in Cvetkovic et al. (1999) and also used in Painter et al. (2008). In these references, however, it is denoted by the parameter β.

Matrix diffusion is caused by solute random movement, which, in the presence of concentration gradients, causes a net movement of solute. In SR-PSU it is assumed that the connectivity of the matrix pore space is not physically limited beyond the limitation imposed by the spacing between adjacent flow bearing fractures. Thus, it is the fracture spacing (strictly half-spacing) that governs the maximum penetration depth. Depths of a few centimetres are frequently sufficient to make matrix diffusion an effective retarding process provided the F-factor is sufficiently high that diffusive uptake to the rock matrix is significant. After entering the pore system, the solutes may sorb on the extensive pore surfaces. For non-sorbing species, it is also important that matrix diffusion extends the residence time, increasing the time for radioactive decay. Since the mineral surfaces are most often negatively charged under natural conditions, there is a repulsion of negatively charged ions close to the surfaces, which can decrease matrix diffusion. Another process which could potentially decrease matrix uptake is pore clogging caused by the precipitation of secondary minerals due to reactive processes involving cementitious leachate 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 such as 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 at repository depth in the bedrock are normally mildly to moderately reducing. If the redox potential is sufficiently reducing the retention of some redox-sensitive radioelements may be enhanced owing to the reduced mobility of these substances under such conditions.

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 with regard to their impact on groundwater bulk chemistry. This is also largely true for uranium despite the significant inventory in the waste. The large reducing capacity of iron oxides, such as magnetite, and the low oxidative capacity of the groundwater for the hydrogeochemical conditions expected at the site, results in only a very small release of uranium into the far field. As a consequence, the influence of radionuclides on other substances in the geosphere is negligible.

In some cases, it should be taken into account that a radioelement can migrate together with much more abundant inactive isotopes of the same element (i.e. ^{90}Sr with ^{88}Sr). It is possible that radionuclides first precipitate and later, following a change in groundwater chemistry, rapidly dissolve. However, owing to the geochemical stability (through the buffering capacity of the geosphere), the potential for such transient episodes decreases with increasing depth.

The attachment of radionuclides to minute particles, or carrier colloids, in groundwater involves a large variety of possible processes. Site investigations have revealed typically low concentrations of natural carrier colloids and other particles suspended in groundwater, suggesting only minor relevance for migration of radionuclides in natural groundwaters. A more important concern is the possibility of bentonite colloids formed by erosion of backfill and buffer materials. This is discussed in more detail in **Barrier process report**. The attachment can be reversible or irreversible, and the particles can be mobile or immobile. Furthermore, the size and composition of particles can change with time, and microbes add complexity to the system with their metabolic processes. The largest particles are mechanically filtered within a fracture, whereas the smallest ones are transported with the water flow. Owing to the existence of a hydrodynamic boundary layer in the fracture (and the preferential transport of colloids in the non-boundary layer fluid), this can result in radioelements being advected at a faster rate than would be predicted for purely dissolved concentrations in flowing water.

6.2.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 6-3 outlines how the process is influenced by the defined geosphere variables, while Table 6-4 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. In Section 6.2.7, this handling is further detailed in a discussion provided by the SR-PSU team.

Explanation of Table 6-3

Temperature in bedrock

Temperature influences all categories of chemical reactions that are likely to occur in groundwater as well as surface chemical processes (sorption and solid phase equilibria). As a general rule, equilibrium chemical reactions described as being exothermic (producing heat) are promoted by reduced temperatures while endothermic reactions are hindered. Temperature can also have an indirect impact on sorption by altering the species distribution of the solutes in groundwater. By altering the thermodynamic conditions for solution speciation reactions, competitive effects are therefore subtly altered. This is discussed in more detail in Section 5.3.

Groundwater flow

Groundwater flow may indirectly affect sorption, by way of affecting the groundwater composition. This might occur, for example, as a result of hydrodynamic mixing of leachate from structures and stray materials with groundwater flowing through the fracture system (see also Section 5.3).

Groundwater pressure

The groundwater pressure has a direct effect on sorption by its influence on the equilibrium constant in sorption/desorption reactions. It also has an indirect influence by way of its impact on groundwater composition via the same mechanism (i.e. it exerts an influence on chemical speciation and solubilities of gases and minerals). The impact of pressure effects, however, is deemed to be very small and can be reasonably neglected in SR-PSU.

Table 6-3. Direct influences of defined geosphere variables on the process "transport of radionuclides in the water phase" and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 6.2.7)
Temperature in bedrock	Yes. Direct impact on chemical equilibria, indirectly through impact on viscosity and density, which affects flow.	E/O	Process not relevant, as radionuclides are not released to the geosphere.
		T/P/G	Sorption coefficients and matrix diffusivities chosen for relevant temperature conditions.
Groundwater flow	Yes. Groundwater flow governs transport.	E/O	Process not relevant, as radionuclides are not released to the geosphere.
		T/P/G	Flow paths, Darcy flux, flow-related transport resistance, advective travel time taken from site-specific groundwater flow modelling, see Chapter 3.
Groundwater pressure	No, but indirectly since pressure affects groundwater flow.	All	See influence of *Groundwater pressure* on *Groundwater flow* in Chapter 3.
Gas phase flow	No, but indirectly since gas phase flow affects groundwater flow.	All	See influence of *Gas phase flow* on *Groundwater flow* in Section 3.3.
Repository geometry	Yes. Repository geometry affects distribution and characteristics of flow paths, and hence transport, to the surface.	E/O	Process not relevant, as radionuclides are not released to the geosphere.
		T	Flow paths and characteristics from site-specific groundwater flow modelling where tunnel layout is implemented in the models, see Sections 3.1 and 3.2.
		P/G	See Temperate above. However, repository not explicitly included in groundwater flow model incorporating permafrost and ice sheet.
Fracture and pore geometry	Yes. Fracture network geometry governs flow and hence non-reactive transport characteristics.	E/O	Process not relevant as radionuclides are not released to the geosphere.
		T/P/G	Flow-related transport resistance from site-specific groundwater flow modelling used, see Section 3.2.
Rock stresses	No, but indirectly since stress affects fracture aperture and groundwater flow.	All	See influence of *Rock stress* on *Groundwater flow* in Section 3.2.
Matrix minerals	Yes. For diffusing species, matrix minerals affect sorption behaviour in matrix and also the extent of diffusion.	E/O	Process not relevant, as radionuclides are not released to the geosphere.
		T/G/P	Site-specific porosities and formation factors considered in the selection of matrix porosity and diffusivity, see Section 5-3. Site-specific porosities, rock mineralogy, BET surfaces and stress effects considered in the selection of K_d values, see Section 5.4.
Fracture minerals	Yes. Fracture minerals affect fracture surface sorption and also access to matrix through diffusion.	E/O	Process not relevant, as radionuclides are not released to the geosphere.
		T/G/P	Surface sorption conservatively neglected in safety assessment for the defined modelling scenarios. Changes in accessibility to rock matrix are judged to be insignificant.
Groundwater composition	Yes. Groundwater composition affects speciation of radionuclides, and hence their transport characteristics.	E/O	Process not relevant as radionuclides are not released to the geosphere.
		T/G/P	Site-specific water salinity, pH, redox, organic acids, microbes considered in the selection of sorption and diffusion data, see Section 5.2, 5.3 and 5.5.
Gas composition	No, but indirectly through dissolution in groundwater of some gases (e.g. O_2, CO_2 and H_2), which affects radioelement speciation.	All	See influence of *Gas composition* on *Groundwater composition* in Section 3.3 and 5.5.
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.	E/O	Process not relevant as radionuclides are not released to the geosphere.
		T/G/P	Sorption on structural and stray materials in the geosphere is neglected.
Saturation	No, but indirectly since saturation affects groundwater flow.	All	See influence of *Saturation* on *Groundwater flow* in Section 3.2.

Gas phase flow

Gas phase flow may indirectly affect sorption, by way of affecting the groundwater composition upon dissolution/degassing. Gas phase equilibrium is only indirectly considered through the hypothetical equivalent partial pressure of various gas components (principally CO_2 and O_2) obtained in reaction calculations.

Repository geometry

The repository geometry has no direct effect on sorption although it will have a strong impact on the contact of groundwater with cemetitious materials which will have an impact on the extent and persistence of a high pH plume due to mixing of groundwater with OPC leachate (see also Section 5.3).

Fracture and pore geometry

Fracture and pore geometry determines sorptive surface area, and accessibility of this area via advection or matrix diffusion. Although not directly addressed in radionuclide transport calculations this is implicitly considered in the estimations of F-factors and advective travel times supplied as input data from the Hydrogeological modelling team.

Rock stresses

Rock stresses are not directly considered to affect radionuclide transport.

Matrix minerals

Matrix minerals are considered in the recommendation of site specific K_d values for use in radionuclide transport calculations.

Fracture minerals

Although sorption on fracture minerals may provide additional capacity for radionuclide transport retardation, they are neglected in radionuclide transport calculations by appealing to arguments of conservatism (for the defined radionuclide transport scenarios).

Groundwater composition

Groundwater composition is considered in the recommendation of site specific K_d values for use in radionuclide transport calculations.

Gas composition

Gas phase equilibrium is only indirectly considered through the hypothetical equivalent partial pressure of various gas components (principally CO_2 and O_2) obtained in reaction calculations.

Structural and stray materials

Sorption may also be affected indirectly by structural and stray materials since their degradation can influence groundwater composition. These processes are not directly considered in radionuclide transport calculations, although they are implicitly considered in scenario specific K_d values (i.e. K_d values for high pH conditions) recommended for use in radionuclide transport calculations.

Saturation

Saturation is not directly considered in radionuclide transport calculations since the geosphere is assumed to be fully saturated during the relevant time domains for radionuclide migration.

Table 6-4. Direct influences of the process “transport of radionuclides in the water phase” on the defined geosphere variables, and a short indication of how the influences are handled in safety assessment SR-PSU. Abbreviations: E/O/S = Excavation, operation, and saturation period, T = Temperate climate domain, P = Periglacial climate domain, G = Glacial climate domain, EQ = Earthquake.

Variable	Influence present? Yes/No/Indirect (Description)	Time period/ Climate domain	Indication of handling of influence in safety assessment. (How/If not – Why)
Temperature in bedrock	No. Reactions of trace amounts of radionuclides will not affect bedrock temperature.	All	
Groundwater flow	No. Trace amounts of radionuclides will not affect bulk thermophysical properties of the groundwater or the groundwater flow.	All	
Groundwater pressure	No. Dissolved radionuclides will not affect the groundwater pressure.	All	
Gas phase flow	No. Trace amounts of radionuclides will not affect gas phase flow, even if some radionuclides come out of solution.		
Repository geometry	No. The repository geometry is not affected by transport of radionuclides.	All	
Fracture and pore geometry	No. The amounts of transported radionuclides are negligible in terms of mass, and will not affect the fracture geometry, even upon precipitation.	All	
Rock stresses	No. Radionuclides do not affect rock stresses.	All	
Matrix minerals	Yes. Reactions of radionculides may result in mineral aletrations and changes in speciation of mineral surface groups. However, as radionuclides are in trace amounts these are of negligible significance.	All	
Fracture minerals	Yes. Reactions of radionculides may result in mineral aletrations and changes in speciation of mineral surface groups. However, as radionuclides are in trace amounts these are of negligible significance.	All	.
Groundwater composition	Yes. (Transport of dissolved species affects the water composition. This is of no significance for understanding bulk chemistry, but useful for understanding radionuclide migration).	E/O	Process not relevant, as radionuclides are not released to the geosphere.
		T/P/G	Radionuclide concentration along the flowpaths, and subsequent release to the biosphere i modelled.
Gas composition	Yes. (Degassing of dissolved radionuclides affects the gas composition. This is of no significance for understanding bulk chemistry, but useful for understanding radionuclide migration.)	All	The principal gas forming radionuclide in SR-PSU is ^{14}C (as $^{14}CO_2$ or $^{14}CH_4$). Formation of significant quantities of $^{14}CH_4$ is deemed not to occur under the chemical conditions of the repository environment (**Waste process report**). Existence of a $^{14}CO_2$ gas partial pressure in equilibrium with dissolved ^{14}C carbonate is implicitly considered in groundwater chemistry calculations and does not need to be considered explicitly.
Structural and stray materials	No. Trace amounts of radionuclides will not affect properties of structural and stray materials.	All	
Saturation	No. Solutes do not affect the degree of saturation.	All	

Explanation of Table 6-4

Temperature in bedrock

Transport of radionuclides at the concentration levels envisaged is not expected to affect the energy balance of the groundwater–rock system, and thus will not affect the bedrock temperature.

Groundwater flow

The effect of radionuclide transport on groundwater composition (thus also water viscosity and density) is too small to affect the groundwater flow in any significant way at the concentration levels envisaged.

Groundwater pressure

Transport of radionuclides at the concentration levels envisaged is not expected to affect the groundwater pressure.

Gas phase flow

Transport of radionuclides at the concentration levels envisaged is not expected to affect the flow or bulk composition of any gas phases present.

Repository geometry

Transport of radionuclides does not have any relevant influence on the repository geometry.

Fracture and pore geometry

Transport of radionuclides at the concentration levels envisaged is not expected to affect the geometry of fractures or pore-apertures in any significant way.

Rock stresses

Transport of radionuclides is not expected to affect the stress situation of the bedrock.

Matrix minerals

Transport of radionuclides at the concentration levels envisaged is not expected to affect reactive properties of the matrix minerals in any significant way.

Fracture minerals

Transport of radionuclides at the concentration levels envisaged is not expected to affect reactive properties of the fracture minerals in any significant way.

Groundwater composition

Transport of radionuclides at the concentration levels envisaged is not expected to affect the bulk groundwater composition (here taken to include redox), although it will exert an influence on the total amount of that radionuclide present in the groundwater.

Gas composition

Transport of radionuclides at the concentration levels envisaged is not expected to affect the bulk gas phase composition.

Structural and stray materials

Transport of radionuclides does not have any relevant influence on structural and stray materials.

Saturation

Transport of radionuclides is not expected to affect the degree of saturation in any significant way.

6.2.3 Boundary conditions in SR-PSU

The inner boundary condition is the concentration of radionuclides in the water phase leaving the engineered barriers. This concentration is provided by the near-field radionuclide modelling. The outer boundary is the geosphere–biosphere interface zone, or alternatively, the vertical and/or bottom boundary of the groundwater flow simulation domain.

6.2.4 Model studies/experimental studies

Experimental studies of individual processes are discussed in Section 6.1.4 and 6.2.4. Experimental studies of the combined processes under spatial and temporal scales of relevance for performance assessment applications do not exist. However, on shorter timescales, the TRUE-1 (Winberg et al. 2000, Widestrand et al. 2007, Cvetkovic et al. 2007, Cvetkovic and Cheng 2008) and TRUE Block scale (Poteri et al. 2002, Winberg et al. 2003, Neretnieks and Moreno 2003, Cvetkovic et al. 2010, Cvetkovic and Frampton 2010) experiments have shed light on predictive capability using models based on the same processes as described above. The SKB studies summarised in Löfgren et al. (2007) indicate an adequate understanding of the relevant processes. Other studies of relevance from other national programmes focused on repositories hosted in crystalline rock are Alexander et al. (2009) and Smith et al. (2001).

Model studies for spatial and temporal scales of relevance for safety assessment applications have been performed in earlier performance assessment studies (e.g. SR97, SR-Can (SKB 2006c) and SR-Site (SKB 2011)), but most notably in the Task 6 of the Äspö Task Force on modelling of groundwater flow and transport of solutes (Hodgkinson and Black 2005, Hodgkinson et al. 2009, Gustafson et al. 2009, Moreno and Crawford 2009). There, a comparison has been made between models with a detailed description of processes and more traditional safety assessment models where a higher level of process abstraction is made. Specifically it has been studied how these models scale in time and space when going from typical experimental time and space scales to safety assessment scales. Also, these studies confirm that the processes discussed above are adequate for application to the scales of interest for performance assessment. However, the type of processes that typically dominate tracer experiments (e.g. sorption on fracture surfaces and diffusion into fracture rim zones with subsequent sorption) are not necessarily of interest on the longer timescales.

6.2.5 Natural analogues/observations in nature

Supporting evidence from natural analogues and observations in nature are discussed in conjunction with the individual processes described in Chapter 5. Natural analogue evidence is not directly applicable for the integrated transport model mostly due to the current lack of data, or sometimes poor agreement between natural analogue data and model predictions in the case of high pH conditions (for discussion, see e.g. Alexander et al. 1998). In spite of this, 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. (2000).

6.2.6 Time perspective

Radionuclides in the water phase are not expected to migrate into the geosphere during the excavation and operation period. The reason is that water is pumped out of the caverns, thus creating a hydraulic gradient from the geosphere toward the caverns. A similar situation is thought to prevail during the resaturation phase of the repository. After the saturation period, radionuclide transport in the water phase needs to be accounted for throughout the assessment time frame.

6.2.7 Handling in safety assessment

In this section, the SR-PSU team gives recommendations on how the process of diffusion and radionuclide transport in the rock mass should be handled. The description is divided into two different parts. In the first part, issues concerning different time periods, climate domains, and events are addressed. In the second part, issues concerning the geosphere variables listed in Table 6-3 and Table 6-4 are addressed.

The radionuclide transport calculations in SR-PSU are performed using the Ecolego tool (**Model summary report**), for the whole calculation chain (near-field, geosphere and biosphere). The geosphere is modelled with a compartment model, based on the same conceptual model as the FARF31 code (used by SKB in many earlier assessments). The compartment model implementation allows time-varying parameters to be accounted for. This option is used in SR-PSU as the modelling considers time varying flow parameters (i.e. F-factors and advective travel times) which are used to represent the changes of flow conditions during land-rise. The details of the model implementation are described in the **Radionuclide transport report**.

The model is equivalent to the FARF31 code (when used without time dependent parameters).

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

The process is of no relevance for the excavation and operation period. Concerning SFR-3, no waste is present during excavation. However, the excavation of SFR-3 should be considered when assessing the function of SFR-1 during this period. In any case, during both operation and excavation, water is pumped out of the caverns and as a result, the hydraulic gradients are directed from the geosphere towards the caverns. Radionuclides will therefore not migrate into the geosphere. Transport of radionuclides is deemed to occur only after the repository is fully saturated and assumes direct migration to the surface without passing through adjacent vaults or storage units.

Temperate climate domain

The most detailed analysis of radionuclide transport is performed for the initial temperate climate domain. Within SR-PSU the transport along path lines from individual repository storage units to the biosphere is described (Odén et al. 2014). The flow paths are obtained from groundwater flow modelling, cf. Section 3.1. The results that are transferred from the flow models to Ecolego-FARF31 and MARFA are the flow-related transport resistance and advective travel time from the waste vaults to the biosphere. Thus, flow modelling and transport modelling are decoupled.

The RNT-model solves the transport equations along the one-dimensional path lines (conceptualised as streamtubes) based on a dual porosity description with advection–dispersion in the mobile phase (flowing water) and diffusion into the immobile water in the rock matrix. An exchange term between the two phases is included in the governing equations. A finite penetration depth for radionuclides is assumed in the model (based on fracture half-spacing). In the matrix, the radionuclides are subject to sorption described using the linear equilibrium K_d concept.

The main inputs to the above analysis 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-PSU assessment (**Data report**, SKB 2010c). Also, the repository tunnel layout is needed for assigning starting positions for particles in the groundwater flow model.

Periglacial climate domain

The simulation of groundwater flow during periglacial conditions aims at establishing groundwater flow patterns during the period when the site is subject to permafrost but no ice sheet is present. Radionuclide transport during the periglacial climate domain is handled in a similar manner as for the temperate period, however during the periglacial period the the flow conditions are different as the main part of the ground is expected to be frozen and the recipient of interest is a talik lake.

Glacial climate domain

As resent research (**Climate report**) has shown that glaciation is not expected to occur during the first 100ka after the closure of SFR, no specific hydrological calculations for glacial conditions have been performed within SR-PSU. However the possible effects from releases of the remaining inventory of radionuclides from a repository severely damaged by a late glaciation period has been performed. This calculation case has been examined only for illustrative purposes in simple calculations where no credit is taken for radionuclide transport and retention in the geosphere (**Radionuclide transport report**).

Earthquakes

The potential impact of earthquakes is illustrated by simple calculations where no credit is taken for radionuclide transport and retention in the geosphere. This is motivated by the fact that shear displacement is expected to occur in larger fractures, where the transport resistance is initially low. Furthermore, the retention characteristics of these fractures after the shear displacement event are essentially unknown.

Handling relative to geosphere variables

Temperature in bedrock

Changes in temperature affect flow related migration properties as well as non-flow related migration properties. Flow related migration properties are provided from the hydrogeological modelling; wherein temperature conditions are accounted for through various relations and correlations (see Section 3.1). Also changes in flow patterns due to permafrost are accounted for in the hydrogeological modelling. As permafrost may effectively halt the groundwater flow, it may also halt long-range radionuclide transport.

For non-flow related migration properties (Sections 5.2 and 5.3), the processes and their related data should be described for a reasonable temperature range. The data variability due to varying bedrock temperature is included in the data uncertainty for D_e and K_d given in the **Data report**.

Groundwater flow

Flow related migration properties are provided from the hydrogeological modelling, as accounted for in Section 3.1.7.

Groundwater pressure

Changes in groundwater pressure mainly affect flow related migration properties as provided from the hydrogeological modelling. For non-flow related migration properties (Sections 5.2 and 5.3), the processes and their related data are for practical purposes independent of the groundwater pressure.

Gas phase flow

The gas phase flow only affects the radionuclide transport in the water phase in an indirect manner as it influences the groundwater flow and, to a very minor extent, the contact area between flowing water and stagnant water. Gas phase radionuclides may also dissolve in the water, and thereby become part of the radionuclide modelling in the water phase.

Repository geometry

The repository geometry affects the groundwater flow, and thereby indirectly affects the flow related migration properties. Accordingly, the geometry is used as an input to hydrogeological modelling (see Section 3.1.7). Except for this, the repository geometry is not accounted for in radionuclide transport modelling in the water phase.

Fracture geometry

The large-scale fracture geometry is an input to hydrogeological modelling, and affects the groundwater flow as well as the flow related migration properties. Small-scale (local) fracture geometry may affect the contact area between the flow path and the stagnant water in the porous system of the rock matrix. This has in previous safety assessments (e.g. SKB 2006c) resulted in assigning a channelling factor. However, as suggested in Crawford and Sidborn (2009) solutes may diffuse into stagnant water volumes and from there into the rock matrix. If the F-factor is sufficiently high, a channelling factor may not always be required and the entire fracture plane can then be assumed to function as the contact area between flowing water and the rock microporosity. The same, however, cannot be said for fast flowpaths featuring low F-factors where channelling effects may be very significant and need to be considered.

Rock stresses

Rock stresses may affect the groundwater flow and subsequently, the flow related migration properties (see Section 3.1). Rock stresses are also thought to affect the effective diffusivity (see Section 5.2), and therefore D_e estimates should be representative for in situ stresses. With the exception of this, rock stresses are not accounted for in radionuclide transport modelling in the water phase.

Matrix minerals

Matrix minerals affect non-flow related migration properties. Therefore, the processes and related data (ε_p, D_e, and K_d) must be relevant for the site-specific rock types. It should also be noted that the pore dimensions of characteristic rock types at the site are such that colloidal transport through the rock matrix cannot occur.

Fracture minerals

No account of additional sorption on fracture minerals has been included in the radionuclide transport calculations performed in SR-PSU. This is considered to be a pessimistic approach.

Groundwater composition

The composition affects the viscosity and density of the groundwater. This also affects the groundwater flow (see Section 3.1) and subsequently, the flow related migration properties. The main effect on the non-flow related migration properties is on the sorption partitioning coefficient K_d. Therefore, K_d data must be supplied for relevant groundwater compositions. However in the radionuclide transport modelling, a pessimistic selection of K_d values has been made for practical reasons. Where possible, correlation between major groundwater composition parameters and K_d is provided. It may also be appropriate to provide different sets of data that are only valid under certain conditions. As an alternative, the effect of variation in the water composition on K_d data should be included in the K_d uncertainty range provided in the **Data report**. The groundwater composition only affects D_e to a minor degree, which in SR-PSU is limited to the assignment of lower D_e values for anionic species. In SR-Site it was suggested that the anion exclusion reduction factor is, on average, half an order of magnitude (SKB 2010c, Section 6.8). This can be compared with the assumption of the Finnish programme, where the reduction factor has been suggested to be one order of magnitude (e.g. Valkiainen et al. 1996, Olin et al. 1997). An additional impact of groundwater composition exists for effective diffusivity measurement data derived from in situ electrically based methods. The effect of these processes on D_e has been included in the D_e uncertainty range provided in the **Data report**.

Gas composition

Radionuclides carried in a gas phase may dissolve and become part of the radionuclide inventory transported in the water phase. No account of this has been taken in the radionuclide calculations for SR-PSU. A scenario with release of radionuclides in the gas phase has been evaluated and in this calculation the gas is assumed to reach the biosphere without retardation in the geosphere. This is a pessimistic assumption.

Structural and stray materials

Structural materials may affect the groundwater composition. For example, alkaline leachate from concrete and corrosion of ferrous reinforcing materials may affect the groundwater pH and redox conditions, which primarily affects the K_d data. The K_d data for unaltered groundwater during the various climate domains has therefore been supplied together with corresponding recommendations for high pH conditions. A pessimistic approach of selecting the lowest K_d values over all groundwater compositions and pH values has been chosen for the radionuclide transport calculations.

Saturation

The geosphere is expected to be fully saturated by the time it is possible for radionuclides to escape the repository. The exception is in the very near-surface rock in the case of no, or very limited overburden. In SR-PSU the radionuclide transport through the geosphere is assumed to take place in fully saturated rock along the entire flow path.

6.2.8 Handling of uncertainties

Uncertainties in mechanistic understanding

Uncertainties in the individual processes are discussed in the relevant sections describing each process.

Model simplification uncertainties

The conceptualisation of velocity variations as a dispersion process and its implementation in the compartment model results in some uncertainty. Dispersion/mixing along the individual flow paths is modelled by means of a dispersion term. This is expressed through the dimensionless Peclet number that quantifies the ratio between advective and dispersive transport. The effect of the chosen value on results is small; hence also the effect of the associated uncertainty on results is small. However, it is noted that the approach in the model using the flow path integrated flow-related transport resistance value is based on an assumption of no dispersion. Hence, inclusion of dispersion in the calculations adds to the uncertainty in the sense that an underlying assumption is not fully met.

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 represented, (constant) average 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, for example, P_{32} values or conductive fracture frequency.

In earlier safety assessments (e.g. SR-Site (SKB 2011)), it has been argued in the Radionuclide transport report (SKB 2010f) that no reduction in flow-related transport resistance due to channelling should be applied. This is based on calculations showing that if channelling occurs, there is also diffusion into stagnant water zones next to the channels in the fracture plane. The diffusion into these stagnant water zones is accompanied by subsequent diffusion into the matrix. The formation of stagnant water thus compensates the effects caused by channelling.

Concerning sorption, the uncertainties are more of a mechanistic nature than related to modelling. Specifically, the simplification of adopting the K_d-approach implies uncertainties as discussed in Section 5.4. Furthermore, the process of sorption on colloidal material is associated with relatively large uncertainties. These uncertainties concern whether the process is reversible or not, and the actual concentrations of colloidal materials that are present in the groundwater. The process is of limited relevance for the overall safety of the repository when naturally occurring colloids are considered, since high concentrations of colloidal material rarely occur naturally in the site-specific groundwaters of interest. Bentonite colloids may be generated by erosion of backfill, especially during periods when dilute glacial meltwaters reach repository depth. Although this may have a significant impact on far-field dose rates, it has been neglected in SR-PSU since this process is most likely to occur during time domains when there is not expected to be a significant human presence at the surface and landscape dose factors are consequently much lower at such times.

In RETROCK (2005) it was discussed at some length if the coupling of the individual processes, as embodied though the governing equations implemented as, for example, in FARF31 implies an additional integrated model uncertainty relative to the uncertainty of the individual processes. No such uncertainty was identified.

6.2.9 Adequacy of supporting references

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

6.3 Transport of radionuclides in the gas phase

6.3.1 Overview/general description

The flow of gas in the geosphere is described in Section 3.3. This section describes how radionuclides can be transported by a gas phase.

At the pore-fluid pressure prevailing in a geological 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 6.2.

If a free-gas phase is present, gaseous radionuclides or radionuclides in molecules that are present in volatile or gaseous compounds can partition into the gas phase and be transported with the gas. As indicated in Section 3.3.1, the natural concentrations of dissolved gases are not expected to be sufficient in themselves to form a gas phase at the water pressure prevailing at repository depth. A scenario in which a free-gas phase might form is where the corrosion of metal parts generates bubbles of free gas. Only radionuclides that can exist in the gas phase, either in their own right (e.g. noble gases) or as part of a gaseous compound (e.g. $^{14}CH_4$) 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 groundwaters at repository depth 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. Colloids may also be generated in the bituminised waste. There is thus a possibility of indirect transport of radionuclides with gas bubbles generated in or near the Silo where there is a large amount of bentonite that conceivably could release colloidal particles.

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 3.3.

6.3.2 Dependencies between process and geosphere variables

In this section, dependences between this process and defined geosphere variables that are commonly expected in fractured crystalline rock are outlined. This means that they are applicable for, but not limited to, the host rock at the SFR site in Forsmark. Table 6-5 outlines how the process is influenced by the defined geosphere variables, while Table 6-6 outlines how the process influences the defined geosphere variables. Furthermore it is indicated during what time period, climate domain, or event that the described influence is valid. The influence between the process and each geosphere variable is elaborated upon below. In the rightmost column there is an indication of the handling of the influence in the safety assessment SR-PSU. In Section 6.3.7, this handling is elaborated upon in a discussion provided by the SR-PSU team.

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. During operation, gas is vented but this is not included in the long-term safety assessment. Furthermore, gas production has essentially ceased before the first periglacial and glacial periods. Accordingly, there is no significant source of gaseous radionuclides during such periods.

Table 6-5. Direct influences of defined geosphere variables on the process "Transport of radionuclides in the gas phase" and a short indication of how the influences are handled in safety assessment SR-PSU.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 6.3.7)
Temperature in bedrock	Yes.	All	Influence mainly via solubility. Not considered in calculations.
Groundwater flow	No, but indirect through: Gas phase flow.	All	Not considered in calculations.
Groundwater pressure	No, but indirect through: Gas composition and gas phase flow.	All	Not considered in calculations.
Gas phase flow	Yes.	All	The residence time of gas in the geosphere is assumed to be zero. Exit locations are assumed directly above the repository.
Repository geometry	No, but indirect through: Gas phase flow.	All	Not considered in calculations.
Fracture and pore geometry	No, but indirect through: Gas phase flow.	All	Not considered in calculations.
Rock stresses	No, but indirect through: Gas phase flow.	All	Not considered in calculations.
Matrix minerals	No, but indirectly through: Gas composition.	All	Not considered in calculations.
Fracture minerals	No, but indirectly through: Gas composition.	All	Not considered in calculations.
Groundwater composition	No, but indirectly through: Gas composition.	All	Dissolved radioactive compounds can degas. The impact is small and is neglected. Gaseous compounds ($^{14}CO_2$) may dissolve to a degree depending on the groundwater composition. This is pessimistically neglected in calculations.
Gas composition	Yes.	All	Dissolved radioactive compounds can degas and colloids may attach to gas bubble surface. The impact is small and is neglected. Gaseous compounds ($^{14}CO_2$) may dissolve. This is pessimistically neglected in calculations.
Structural and stray materials	No, but indirectly through: Gas composition and gas phase flow.	All	Not considered in calculations.
Saturation	No, but indirectly through: Gas phase flow.	All	Not considered in calculations.

Explanation of Table 6-5

Temperature in bedrock

The bedrock temperature affects the properties of the gas (viscosity, density, and gas solubility) and therefore the gas flow. The overall gas flow in turn affects the flow of gaseous radionuclides, assumed to be in trace concentrations. The temperature also has a direct influence on the gaseous radionuclides, as their solubility is affected.

Groundwater flow

The groundwater flow and overall gas phase flow are coupled (see Chapter 3.). Accordingly, the flow of gaseous radionuclides is indirectly affected.

Groundwater pressure

The groundwater pressure affects the groundwater flow, and thus indirectly the flow of gases (see Section 3.3.2) and gaseous radionuclides. A change in pressure will change the gas volume and affect the proportions between a component in the gas phase and gas dissolved in water. For the expected differences in hydraulic pressure during the period when gas is produced, the effect is negligible.

Gas phase flow

The overall gas phase flow governs the transport of radionuclides in gas phase.

Repository geometry

The repository geometry could influence the distribution pattern of the gas phase flow, and indirectly of radionuclides in gas phase leaving the near field.

Fracture and pore geometry

The fracture and pore geometry affects the gas phase flow pattern (see Section 3.3.2) and subsequently the flow of gaseous radionuclides. Also, gaseous radionuclides may dissolve in the water in the fracture and diffuse into the rock matrix.

Rock stresses

The rock stresses may affect fracture and pore geometry and therefore the gas phase flow (see Section 3.3.2) and subsequently the flow of gaseous radionuclides.

Matrix minerals

Gaseous radionuclides may dissolve in the groundwater, which will lower their concentration in the gas phase. Subsequently the dissolved gasses may diffuse into the rock matrix, where the dissolved gasses could interact with matrix minerals.

Fracture minerals

Gaseous radionuclides may dissolve in the groundwater, which will lower their concentration in the gas phase. Subsequently the dissolved gases may interact with fracture minerals. Radioactive $^{14}CO_2$ could react with minerals and dissolve as CO_3^{2-} or precipitate. Effect is deemed to be marginal.

Groundwater composition

The groundwater composition will affect the partitioning of some radionuclides between the water phase and gas phase. Accordingly the transport of gaseous radionuclides is indirectly affected. This effect is deemed to be marginal.

Gas composition

The concentration of gaseous radionuclides in the gas phase affects the potential for radionuclide transport in the gas phase. Also the gas concentration could affect the chemical state of gaseous radionuclides, as well as the partitioning of the radionuclides between the water phase and gas phase. This effect is deemed to be marginal.

Colloids attach to the water/gas interface. Only large swarms of very small bubbles can potentially carry appreciable amounts of colloids. The gas escape through the rock fractures is expected to be through connected gas channels. Such flow paths will have a small surface area for colloid attachment and cannot be expected to detach the colloids from the gas. The only source of colloids for the groundwater compositions expected during temperate conditions, that could conceivable attach to the bubbles in the repository, are from the bentonite surrounding the repository. Even so, the gas would have to have been pressed through the bentonite to tear away the smectite particles from the bentonite as the gas forms bubbles when emerging in the free-water. The construction of the silo top is such that gas is allowed to escape without generating high pressure that could damage the walls. As the Silo is vented no gas flows through the bentonite is expected.

The situation could be different after glacial conditions when melting ice water contacts the bentonite. Then bentonite may spontaneously release colloids. However, by this time gas generation has long since ceased.

Structural and stray materials

In the near-field rock adjacent to the repository, cementitious grouting may react with dissolved ^{14}C bound carbon dioxide.

Saturation

The saturation affects the gas phase flow (see Section 3.3.2). Accordingly the transport of radionuclides in the gas phase is indirectly affected. This effect is deemed to be marginal during saturated conditions.

Table 6-6. Influences of the process “Transport of radionuclides in the gas phase” on defined geosphere variables, and a short indication of how theseinfluences are handled in safety assessment.

Variable	Direct influence present? Yes/No/No, but indirectly through: variable or process	Time period or event	Handling of influence in safety assessment (as further described in Section 6.3.7)
Temperature in bedrock	No.	All	–
Groundwater flow	No.	All	–
Groundwater pressure	No.	All	–
Gas phase flow	No.	All	–
Repository geometry	No.	All	–
Fracture and pore geometry	No.	All	–
Rock stresses	No.	All	–
Matrix minerals	No.	All	–
Fracture minerals	No.	All	–
Groundwater composition	Yes.	All	Dissolution of radioactive gasses is neglected in calculations of liquid phase radionuclide transport.
Gas composition	Yes.	All	No modelling of the gas composition in the geosphere is performed.
Structural and stray materials	No.	All	–
Saturation	No.	All	–

Explanation of Table 6-6

Temperature in bedrock

Radionuclides in gas phase exist in trace concentrations and have an insignificant effect on heat transport.

Groundwater flow

Radionuclides in gas phase exist in trace concentrations and have an insignificant effect on groundwater flow.

Groundwater pressure

Radionuclides in gas phase exist in trace concentrations and have an insignificant effect on groundwater pressure.

Gas phase flow

Radionuclides in gas phase exist in trace concentrations that are too low to affect gas properties and, hence, gas phase flow.

Repository geometry

The transport of radionuclides in the gas phase does not affect repository geometry.

Fracture and pore geometry

Radionuclides in gas phase exist in trace concentrations that are too low to contribute to effects that may alter the fracture and pore geometry.

Rock stresses

Radionuclides in gas phase exist in trace concentrations that are too low to contribute to effects that may alter the rock stresses.

Matrix minerals

Radionuclides in gas phase will not affect matrix minerals. Even if the radionuclides dissolve, their concentrations are too low to affect matrix minerals in any significant manner. However dissolved carbon dioxide will diffuse into the matrix pores and can react with minerals to either form bicarbonate or carbonate ions or precipitate as some mineral e.g. calcium carbonate. This will not affect the matrix minerals noticeably but will deplete the gas from a volatile radioactive compound.

Fracture minerals

Radionuclides in gas phase will not affect fracture minerals. Even if the radionuclides dissolve, their concentrations are too low to affect fracture minerals in any significant manner. See also above.

Groundwater composition

Solutes transported in gas phase may dissolve, and hence affect the groundwater composition. Even though only trace amounts of radionuclides may be dissolved in the groundwater, it may be important to keep track of these amounts.

Gas composition

Transport of gaseous radionuclides can modify the gas composition. Even though the gaseous radionuclides only contribute to the gas concentration by trace amounts, it may be important to keep track of these amounts.

Structural and stray materials

Radionuclides in gas phase exist in trace concentrations and have an insignificant effect on structural and stray materials.

Saturation

Radionuclides in gas phase exist in trace concentrations and have an insignificant effect on the saturation.

6.3.3 Boundary conditions

The magnitude and characteristics of the gas-phase flow are the principal controlling factors in the transport of radionuclides in the gas phase.

The additional boundary conditions required are those to determine the concentrations of the radionuclides in the gas phase. This may include the concentration in the gas stream leaving the near field. It could also include the concentrations of the radionuclides in groundwater in contact with the gas stream; these radionuclides may partition into the gas stream.

The outer boundary is provided by the geosphere–biosphere interface zone (it is assumed that the gas flow will be predominantly vertical, unless forced to migrate laterally by some horizontal low permeability or capillary barrier). If, as expected, the flow is advection dominated, the variation of conditions at the surface, within the range that is credible, will not have a significant effect on transport of radionuclides by gases to the surface. Some radionuclide-containing compounds may be transformed to other compounds during their migration to the surface. For example methane could be oxidised to carbon dioxide when migrating through oxidising water near 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. Furthermore, the carrying capacity will be directly proportional to the amount of colloidal particles carried by the gas.

6.3.4 Model studies/experimental studies

Transport of components of a gas phase through porous materials is a well understood process, both experimentally and theoretically. Detailed modelling of the gas flowpaths in fracture networks is not attempted in SR-PSU. 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 to be relatively straightforward. There is some difficulty in assessing the extent to which components in the gas phase may partition into the water phase, arising mainly from the difficulty in determining how much groundwater the migrating gas comes into contact with and on the magnitude of the rate of mass transfer. Characterising details of the gas-phase flow itself, especially in fracture networks, is, however, the main assessment difficulty, as discussed in Section 3.3. The want of the detailed knowledge can be bypassed with the assumption that the gas carrying the radionuclides rapidly reaches the biosphere and release the nuclides there.

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 in a KBS-3 repository 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 spent fuel. The particles were assumed to remain irreversibly bound to the bubbles, while all gas was assumed to reach the ground surface. The actinides remained irreversibly bound to the clay particles, whereas caesium and strontium desorbed from the bentonite clay and underwent matrix diffusion combined with sorption during transport through the rock.
The results of the calculations showed that the releases to the biosphere were very limited for all radionuclides even with these pessimistic assumptions.

The migration of a free gas through an otherwise water-saturated sparse fracture network will take place along channels controlled by the geometry of the connected fracture network and the spatial variability of fracture apertures. Gas-phase flow paths are often subject to instabilities, with a free gas pathway collapsing and reforming, resulting in the formation of separated bubbles, known as Hele-Shaw bubbles. Characteristics of gas transport through single water-saturated fractures have been examined in a number of laboratory experiments and modelling studies (see, for example, Hoch et al. (2001) and Rodwell et al. (1999)). The capacity for gas migration through the fractured rock at Forsmark was considered as part of the SR-Can assessment (Hartley et al. 2006).

6.3.5 Natural analogues/observations in nature

Attempts have been made to identify transport of substances through the geosphere as gases or attached to gas bubbles. Undoubtedly, near the surface, gas-phase transport occurs from below the water table in some areas (leaving aside volcanic systems), but there can be difficulty in determining whether gas-phase transport started at depth or whether gases were transported in solution at depth and only formed a separate gas phase closer to the surface. A review of "geogas" migration can be found in Goodfield and Rodwell (1998) and the references therein, and discussion can also be found in Rodwell (2000). Practically all escaping gas reaches the biosphere through specific faults. Natural analogue studies have not yet contributed significantly to the validation of assessments of gas migration from a repository.

6.3.6 Time perspective

All timescales, 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. Gas production is expected to have ceased after thousands to ten thousand years. When generation of volatile components decreases, gas bubbles will cease to form because the components can diffuse away in the water before the pressure reaches saturation pressure at repository depth.

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.

6.3.7 Handling in the safety assessment

In this section, the SR-PSU team gives recommendations on how to handle the process of transport of radionuclides in the gas phase. The description of the handling is divided into two different parts. Firstly, issues concerning different time periods, climate domains, and events are addressed. Secondly, issues concerning each of the geosphere variables of Table 6-5 and Table 6-6 are addressed.

Handling relative to time periods, climate domains, and events

Excavation/operation/re-saturation period

Radioactive gases formed before repository closure will not enter the geosphere, as the repository is vented. Describing this venting is not part of the long-term safety assessment. It will be not long after repository closure before gas bubbles form, primarily by corrosion of aluminium in the waste. The transport of radioactive gasses during the re-saturation period is handled in the same manner as during periods of temperate climate domain (see below).

Periods of temperate climate domain

In the safety assessment, transport in the gas phase is treated as a short circuit of the repository to the biosphere, i.e. transport through the geosphere is neglected. This means that the assumed residence time is zero and that there is no retention in the geosphere. Furthermore, the exit locations for gaseous radionuclide release are assumed to be directly above the repository. 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.

Periods of the periglacial climate domain

See handling of temperate climate domain (although gas production has essentially ceased at times of the first period of the periglacial climate domain).

Periods of the glacial climate domain

Gas production has ceased at times of the first period of the glacial climate domain.

Earthquakes

The potential impact of earthquakes is neglected since transport in the gas phase is already treated as a short circuit of the repository with the biosphere. Therefore, in the event of an earthquake the handling is the same as described above in handling of temperate climate domain.

Handling relative to geosphere variables

The factors that determine the assumed transport of radioactive gasses to the surface system are their production rate and composition in the repository. In the simplistic approach taken when assessing transport of radioactive gas in the geosphere, which is to short circuit the geosphere, none of the geosphere variables in Table 6-5 and Table 6-6 are considered. Furthermore, the radioactive components in the gas are only present in trace amounts and do not influence any of the geosphere variables, with the exception of gas composition and groundwater composition. Accordingly, only these two geosphere variables are discussed below.

Groundwater composition

The partitioning of some radionuclides between the water phase and gas phase affects the groundwater composition, by either adding or removing radionuclides from the liquid phase. However, it is judged that this partitioning is insignificant and therefore this is not considered when modelling liquid phase radionuclide transport.

Gas composition

The presence of trace amounts of radioactive components in the gas influences the gas composition. However, as results of the simplified modelling in SR-PSU, the gas composition in the geosphere is not explicitly modelled. Only the total amounts of gaseous radionuclides assumed to be transported through the geosphere are estimated.

The degassing of liquid phase radionuclides into gaseous radionuclides may lead to a loss of retention capacity of the geosphere. A similar effect could occur as result of decay and subsequent degassing (Ra-226 to Rn-222). However, these processes are judged to have an insignificant influence on repository safety and are neglected.

6.3.8 Handling of 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, because gas bubbles have a very limited carrying capacity for colloids and small gas bubbles are very likely to coalesce during their transport through the fractures in the rock. When they coalesce, the surface area of the gas decreases and the attached colloids will remain behind.

Model simplification uncertainties

The consequences of the transport of radionuclides by migrating gas are assessed using a model that neglects the rate of transport through the geosphere – the geosphere is effectively short circuited, with gas generated at the repository being approximated as moving directly into the biosphere.

This is a gross simplification of the transport process, but is a robust treatment for evaluation of the consequences. The main approximation made in this approach is neglecting the fraction of the generated gas that dissolves in the groundwater and may then have a significant travel time. Neglecting the travel time of the free gas is expected to be a minor approximation, because the travel time will be short. However, for short lived nuclides such as e.g. ^{222}Rn, the assumption of a zero travel time in the gas phase may be pessimistic since decay could be important.

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 formation and release of radionuclides in gaseous form.

A major uncertainty lies in the fate of the radioactive ^{14}C. In the waste it exists as inorganic carbonate and as bound in organic compounds. Some of it may already originally be present as $^{14}CH_4$, which is a volatile gas. Due to uncertainties in processes occurring in the repository (see the **Waste process report** and the **Barrier process report**), it is uncertain in what form gaseous C-14 compounds will enter the geosphere. As the conditions quickly becomes more reducing, going from the re-saturation period to saturated conditions, the fractions of $^{14}CO_2$ versus $^{14}CH_4$ will shift. This uncertainty is handled by pessimistically not accounting for any dissolution or retention in the geosphere. There is also uncertainty in to what extent methane will be oxidised to carbon dioxide (which can dissolve) in the upper part of the geosphere and in the regolith. This provides uncertainty to the question of in what form C-14 compounds enter the surface system.

Assessment of the transport of sorbed radionuclides by gas bubbles is also subject to considerable uncertainty. However, cautious scoping calculations designed to provide an upper bound to the possible radiological impacts from this transport mechanism again show these radiological impacts to be insignificant and therefore the uncertainties do not undermine the safety assessment.

6.3.9 Adequacy of references supporting the handling in SR-PSU

The references are judged to be adequate and sufficient to support the handling in SR-PSU. Based on the general references, sufficiently extensive arguments for supporting the handling in SR-PSU are given in this process report.

7 Summary and conclusions

7.1 Summary of handling of processes in SR-PSU

Table 7-1 summaries the handling of geosphere processes in the safety assessment SR-PSU, as suggested in this report. In the table, the process is associated with a brief description of how it will be handled. In conclusion, the SR-PSU reference evolution, based on current scientific knowledge, includes periods of temperate and periglacial climate domain. Periods of glacial climate domain are included in a what-if safety assessment scenario based on a repetition of the last glacial cycle (**Climate report**). This scenario assumes completely degraded concrete barriers (**Radionuclide transport report**) and no geosphere retention after a glaciated period, is included. Since the barriers are assumed completely degraded, several processes such as "Deformation in intact rock" are not considered.

Table 7-1. Process table describing how processes in the geosphere are handled in SR-PSU.

Process	Handling
Heat transport	The heat flux from the deep geosphere is represented explicitly in modelling of permafrost development at Forsmark.
Freezing	Modelled with coupled climate and 2D permafrost model. Considered in radionuclide transport calculations.
Groundwater flow	Groundwater flow under saturated conditions is modelled. Uniform groundwater density (i.e. not density-driven flow) is assumed at all times and in the permafrost modelling as well.
Gas flow/dissolution	Gas flow is fast compared to groundwater flow and hence gas dissolution is neglected. Gas transport is handled in Section 6.3. Natural (geothermal) gases from the deep geosphere are not expected at these superficial elevations.
Deformation of intact rock	Thermo-mechanical effects expected during the periglacial and glacial domains are neglected during the assessment period. Deformation in the intact rock, due to excavations, is included in stability modelling.
Displacements along existing fractures	Neglected in groundwater flow modelling. Influence on fracture geometry is negligible compared to the overall uncertainty and the simplifications of the fracture network in the models. Fracture displacement is part of the stability modelling that is performed.
Fracturing	Neglected. The models assume an elastic rock block material. The existing fractures are assumed to dominate the groundwater flow.
Erosion/sedimentation in fractures	Insignificant impact in temperate and periglacial domain, compared with the process actions during periods of glacial climate domain.
Advective transport/mixing of dissolved species	Advective transport is handled in SR-PSU. It is included in the modelling, both explicitly in the transport equations for radionuclides and implicitly through streamline, one dimensional modelling for the evolution of the groundwater composition.
Diffusive transport in the rock mass	Diffusive exchange between the flow path and the surrounding stagnant water is included in the equations in the models.
Speciation and sorption	K_d data, with uncertainty ranges, are assumed to be approximately valid, or conservative, for in situ groundwater composition ranges. Different K_d values are given for different speciations as a result of different redox potential ranges, but the most conservative values are chosen.
Reactions groundwater/rock matrix	Not deemed to lead to appreciable changes in rock matrix porosity or mineralogy. Indirectly considered by use of equilibrated groundwater compositions in the solute transport modelling. The fate of matrix minerals is not assessed in SR-PSU.
Dissolution/precipitation of fracture-filling materials	Not accounted for in RN transport modelling. Included in the thermodynamic analysis of groundwater composition.
Microbial processes	The microbial population is expected to remove oxygen in the post-closure phase and lead to anaerobic conditions. Following this, microbial activity is considered to be limited (inhospitable conditions, high pH, low amounts of dissolved organic matter in geosphere) and to have a negligible influence on radionuclide transport.
Degradation of grout	Degradation of the grout can affect the pH of the groundwater. However, the amount of cement in the waste and barrier system greatly exceeds that in the grout; hence, the grout is considered to have a negligible influence.

Process	**Handling**
Colloidal processes	Low concentrations of colloids are expected; hence, the influence of colloids on radionuclide transport has been neglected in the main scenario.
Methane hydrate formation	Neglected. Unfavourable conditions for formation of methane hydrates, hence not expected to be present.
Salt exclusion	Neglected. No density-driven flow, low initial salinities at depths above 200 m, not likely to be induced.
Earth currents	Earth currents (from e.g. electrochemical reactions) are neglected. Surface conductivity effects are indirectly accounted for in assessing site-specific diffusivities. And there are no ore bodies found in the area (i.e. no potential electroferric content).
Speciation of radionuclides	Pessimistic choice of parameters, analysis of sensitivity cases.
Transport of radionuclides in the water phase	Included in radionuclide transport modelling. In some calculation cases, the transport resistance in the geosphere is not taken into account.
Transport of radionuclides in the gas phase	The gas (mainly due to corrosion of steel in the waste) is assumed to escape through the geosphere, without any delay and without causing any damage.

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1346127 ver 1.0	Geometrioptimering av pluggar för förslutning av SFR – Projekt SFR-utbyggnad. (In Swedish.)	SKB, 2013
1395349 ver 1.0	TD06 – Density driven flow	SKB, 2013